Thermodynamics of Certain Refractory Compounds

THERMODYNAMIC TABLES, BIBLIOGRAPHY, AND PROPERTY FILE

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Thermodynamics of Certain Refractory Compounds

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IN COLLABORATION WITH THE CONTRIBUTORS

VOLUME II

Thermodynamic Tables, Bibliography, and Property File

SECTIONS VII, VIII, and IX

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PREFACE

Since 1954, the Thermal & Solid State Branch of the Air Force Materials Laboratory has had a continuing interest in delineating materials-environment interactions under extreme thermal environments. This interest has most frequently resulted in the Air Force sponsorship of research programs aimed at the measurement of certain optical, thermophysical and thermodynamic properties of materials, kinetic studies of materials-environment interactions, the development of improved techniques for making these measurements, and the consolidation of literature data in some of these areas. This compilation spawned from these interests.

The magnitude of this effort, as has probably been the case with most works of this type, was underestimated. The work presented here is thus a contribution rather than a completed effort. It is hoped that others will continue in this effort. Thermodynamics has demonstrated itself as an important theoretical tool for predicting the chemical and physical behavior of materials under diverse environmental conditions. Much basic thermodynamic data have been and are now being obtained from many research programs throughout the world. However there has always been a distinct need for a program staffed by highly specialized personnel to evaluate, integrate, extrapolate and otherwise reduce these data to make them available in an interconsistent form directly useful to scientists and engineers for design purposes. The recent establishment of the National Standard Reference Data Program finally indicates the realization that we can no longer afford to be without such a continuing effort to help support and guide our research.

There are certain unique features to this work which have not generally been characteristic of other works of this type or at least not in this degree of detail or in this combination. It is believed that these are desirable features and should be considered in any future work of this type. The user's right to disagree has been profusely aided and abetted since the details of the critical analysis leading to the choice of accepted values are presented. Accuracy estimates are listed for most of the tabulated values. The fact that many of the tables extend to 6000°K and contain tabulation of data at close intervals of temperature is considered a great advantage. The program served as a proving ground for many computer techniques whose impact in the information generation, storage, and retrieval areas are yet to be felt.

The help of Mr. Edmund J. Rolinski and Dr. Emile Rutner of the Thermal & Solid State Branch is gratefully acknowledged as are the unknown visionaries in the higher echelons of the Department of Defense who assigned the special funds for the initiation of this effort. The thanks of the Air Force, the U. S. Government and the scientific community are due to the collaborators and contributors to this compilation. Special gratitude is due to Messrs. Hyman Marcus, Jules I. Wittebort and Leo F. Salzberg whose vision, faith, cooperation, patience and understanding were essential in carrying this work to this point.

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FOREWORD

This publication is based on a final report (ASD-TR-61-260 Pt. II, 1964) prepared by the Research and Advanced Development Division of the Avco Corporation on Contract AF33(657)-8223 under Project No. 7360, The Chemistry and Physics of Materials: Task No. 736001, Thermodynamics and Heat Transfer. The work was administered under the direction of the Materials Physics Division of the Air Force Materials Laboratory, Research and Technology Division; the RTD monitor on the program was Mr. Paul Dimiduk of the Thermophysics Section. The data reported herein was compiled between 1 June 1962 and 31 December 1963. This work includes a study of the thermodynamics of the borides, carbides, nitrides, and oxides of 31 elements in the temperature range from 0° to 6000°K. The elements are (a) group II A -- beryllium, magnesium, calcium, and strontium; (b) group III B -- scandium, yttrium, and lanthanum, (c) group IV A -- silicon; (d) group IV B -- titanium, zirconium, and hafnium, (e) group V B -- vanadium, niobium, and tantalum; (f) group VI B -- chromium, molybdenum, and tungsten; (g) group VII B -- manganese, technetium, and rhenium; (h) group VIII -- rhodium, osmium, iridium, and platinum; (i) rare earths -- cerium, neodymium, samarium, gadolinium, and dysprosium; and (j) actinides -- uranium and thorium. More than 160 thermodynamic tables, together with comprehensive discussions, have been prepared. The work has been summarized in two volumes.

Volume 1 (published separately, 690 pp, 1966) presents a summary of the techniques used to analyze thermodynamic data and gives the data analyses for refractories considered. Volume 2 (this book) is a compilation of thermodynamic tables generated on this project. It also contains a bibliography and property file. The latter is essentially a subject index for use with the bibliography.

This work has been the result of the efforts of a group of scientists, including Doctors H. L. Schick, D. F. Anthrop, R. J. Barriault, R. E. Dreikorn, R. C. Feber, M. Griffel, C. H Leigh, M. B. Panish, and C. H. Ward. Project Directors were R. J. Barriault (deceased June 1962), C. H. Leigh (June to December 1962), and H. L. Schick (December 1962 to December 1963). The contributions of different scientists can be identified by reference to the thermodynamic tables of Volume 2. Each of these tables is labeled with the initials of the responsible scientist and the approximate date of the analysis. The corresponding discussion in Volume 1 was also prepared by the same scientist.

His fellow co-workers wish to express their feeling of loss at the untimely passing of Dr. Roland J. Barriault at the beginning of this project in June, 1962. His enthusiasm and leadership were invaluable in a previous contract, AF 33 (616)-7327.

Prof. W. L. Klemperer of Harvard University has acted as consultant on spectroscopic and thermodynamic problems.

Many individuals located throughout the world have been kind enough to provide information to assist this work. An effort has been made to acknowledge such help below. Any omissions are entirely accidental.

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FOREWORD

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FOREWORD

Several scientific meetings have provided opportunity for many valuable discussions. They include:

1. A colloquium on diborides held at Arthur D. Little Company under A. D. Little-Manlabs sponsorship in January 1963.

2. An NRC-OCT conference on critical tables of thermodynamic data held at the National Academy of Science on 14-15 March 1963 under the dual chairmanship of Prof. E. Westrum and Dr. G. Waddington.

3. The Stanford Research Institute Symposium on High Temperature Technology at Asilomar, California, in September 1963.

4. A JANAF Thermochemical Panel Meeting in New York City on 5-7 November 1963.

The cooperation of the library staffs at the Massachusetts Institute of Technology, the Cambridge Research Laboratories at Hanscom Field, The New York office of the Atomic Energy Commission, the Division of Technical Information Extension at Oak Ridge, and Avco RAD has been invaluable.

Analyses were aided by the work of the following summer students at Avco RAD: Messrs. J. Hopps (Boston University) and K. Spears (University of Kansas).

Computer and associated programming were aided by the work of Messrs. W. Duffy, E. Levine, J. Paskalides, L. Reid, E. Vancor, and others.

Bibliography preparation, computations, and general assistance with computer facilities were provided by Miss Charlotte Topliffe, and Messrs. D. V. LaRosa, W. L. Perry, W. Wise, G. Costas, G. Hitchcock, and K. Campbell.

Especially valuable throughout this project has been the wide range of help given by Mrs. Patricia Topham, Mrs. Irene A. Hutnick, and Messrs. D. V. LaRosa and L. I. Rose.

The work reported herein was performed at Avco RAD with the help of all levels of management. Dr. M. E. Malin (Vice-President of Research) showed a continuing interest in the progress of this work.

One of us (H. L. Schick) would also like to express appreciation to Mr. R. Capiaux of Lockheed Missiles and Space Company for support in the final stages of publishing this document.

Vol. 2. Thermodynamic Tables, Bibliography, and Property File (Sections VII, VIII, and IX)

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VII. THERMODYNAMIC TABLES

This document (volume 2) is made up of thermodynamic tables compiled during this project. In addition, any tables from an earlier project[1] which have not been revised during the present work are included in this volume. Hence, the present volume is a complete compilation of the latest tables generated on both projects.

For the user who wishes to know only the important source data, a brief summary is provided on the back of each table. This summary has been patterned after that of the JANAF thermochemical tables. The brief summaries on the backs of these tables are necessarily very sketchy and only refer to data actually used in producing the tables. For the user who wishes a complete background of all data considered in the analyses prior to table preparation, it is necessary that the data analyses of volume 1 be consulted.[2] Data analyses for tables carried over from the previous contract may be found in the earlier work.[1]

For many of the tables included herein, uncertainty estimates have been provided. These uncertainty estimates (when included) always physically follow the tables to which they refer. The estimates serve two purposes:

1. They provide rough guides to the accuracy of the data tabulated. However because of the wide range in quality of thermodynamic data reported in the literature, it is often difficult to give a reliable estimate of the uncertainty. In some cases, the present estimates may do injustice to very precise data and similarly in other cases the opposite may occur. However, overall, the present estimates are a rough guide to the quality of the data.

2. For the casual user who may feel that data tabulated to three significant figures have this accuracy, the uncertainty estimates provide a more realistic appraisal of the situation.

The order in which the tables are placed is according to the modified Hill[3] indexing system for chemical compounds as used by the JANAF Thermochemical Panel Compilation,[4] Chemical Abstracts, and the Classification Division of the U. S. Patent Office. In the upper right-hand corner of each table is an alphabetic arrangement of the atomic symbols in the chemical formula. The order of the tables is alphabetic according to this compound symbol except for carbon compounds which include the very large organic category. In carbon compounds, the elemental symbol "C" always comes first, immediately followed by "H" if hydrogen is present. The other elemental symbols in carbon compounds then

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follow in their regular order. The numbers of atoms of the elements in the compound play a secondary role in determining the tables' positions. Their influence is subordinate to the order in which the atomic symbols occur in the compound symbol. For example, any compound symbol containing "C_2" would come after all others containing "C," regardless of any other element symbols the compound symbol might contain. Reference state and condensed phase tables have been placed before ideal gas tables.

Solid lines with double entries have been used to designate primary transitions, such as solid-state changes, melting points, and normal boiling points, in reference state and condensed phase tables. Dotted lines have been used in the corresponding places in ideal gas tables to indicate discontinuities in the heats of formation of the gases due to the primary transitions in the reference-state phases. Since primary transitions in condensed phases of compounds are not reflected as discontinuities in heats of formation of the corresponding ideal gases, double entries have not been included at such temperatures in ideal gas tables of compounds. Double entries with no lines have been used in tables of compounds to indicate discontinuities in heats of formation due to transitions in the elements.

Two indexes to the tables of this section follow. The filing order presented in tabular form shows the arrangement of tables exactly as they appear (tables 89 to 250). A second index arranged alphabetically can be used for ease in locating a given table.

REFERENCES FOR SECTION VII

1. Barriault, R. J. et al, Thermodynamics of Certain Refractory Compounds, ASD TR 61-260, Pt. I, Vol. 1 (May 1962).

2. Schick, H. L. et al, Thermodynamics of Certain Refractory Compounds, ASD TR 61-260. Pt. II Vol. 1 (1964), present work.

3. Hill, E. A., J. Am. Chem. Soc. 22, 478 (1900).

4. Dergazarian, T. E. et al, JANAF Interim Thermochemical Tables, Vols. 1 and 2, Dow Chem. Co., Midland, Mich. (31 December 1960).

THE THERMODYNAMIC TABLES*

Table	Title	Conventional Formula	Filing Order
	Boron		
89	Reference State	B	B
90	Ideal Monatomic Gas	B	B
	Hafnium Diboride		
91	Condensed Phase	HfB_2	B_2Hf
	Niobium Diboride		
92	Condensed Phase	NbB_2	B_2Nb
	Tantalum Diboride		
93	Condensed Phase	TaB_2	B_2Ta
	Titanium Diboride		
94	Condensed Phase	TiB_2	B_2Ti
	Zirconium Diboride		
95	Condensed Phase	ZrB_2	B_2Zr
	Beryllium		
96	Reference State	Be	Be
97	Ideal Monatomic Gas	Be	Be
	Beryllium Oxide		
98	Condensed Phase	BeO	BeO
99	Ideal Molecular Gas	BeO	BeO
	Beryllium Carbide		
100	Condensed Phase	Be_2C	Be_2C
	Dimeric Beryllium Oxide		
101	Ideal Molecular Gas	Be_2O_2	Be_2O_2
	Beryllium Nitride		
102	Condensed Phase	Be_3N_2	Be_3N_2
	Trimeric Beryllium Oxide		
103	Ideal Molecular Gas	Be_3O_3	Be_3O_3

Table	Title	Conventional Formula	Filing Order
104	Tetrameric Beryllium Oxide Ideal Molecular Gas	Be_4O_4	Be_4O_4
105	Pentameric Beryllium Oxide Ideal Molecular Gas	Be_5O_5	Be_5O_5
106	Hexameric Beryllium Oxide Ideal Molecular Gas	Be_6O_6	Be_6O_6
	Carbon		
107	Reference State	C	C
108	Ideal Monatomic Gas	C	C
109	Hafnium Carbide Condensed Phase	HfC	CHf
110	Dimolybdenum Carbide Condensed Phase	Mo_2C	CMo_2
111	Niobium Carbide Condensed Phase	NbC	CNb
112	Diniobium Carbide Condensed Phase	Nb_2C	CNb_2
113	Silicon Carbide Condensed Phase	SiC	CSi
114	Tantalum Carbide Condensed Phase	TaC	CTa
115	Ditantalum Carbide Condensed Phase	Ta_2C	CTa_2
116	Thorium Carbide Condensed Phase	ThC	CTh
117	Titanium Carbide Condensed Phase	TiC	CTi
118	Tungsten Carbide Condensed Phase	WC	CW

Table	Title	Conventional Formula	Filing Order
	Ditungsten Carbide		
119	Condensed Phase	W_2C	CW_2
	Zirconium Carbide		
120	Condensed Phase	ZrC	CZr
	Diatomic Carbon		
121	Ideal Molecular Gas	C_2	C_2
	Trimolybdenum Dicarbide		
122	Condensed Phase	Mo_3C_2	C_2Mo_3
	Thorium Dicarbide		
123	Condensed Phase	ThC_2	C_2Th
124	Ideal Molecular Gas	ThC_2	C_2Th
	Triatomic Carbon		
125	Ideal Molecular Gas	C_3	C_3
	Calcium		
126	Reference State	Ca	Ca
127	Ideal Monatomic Gas	Ca	Ca
	Calcium Oxide		
128	Condensed Phase	CaO	CaO
129	Ideal Molecular Gas	CaO	CaO
	Cerium		
130	Reference State	Ce	Ce
131	Ideal Monatomic Gas	Ce	Ce
	Cerium Oxide		
132	Ideal Molecular Gas	CeO	CeO
	Chromium		
133	Reference State	Cr	Cr
134	Ideal Monatomic Gas	Cr	Cr
	Chromium Monoxide		
135	Ideal Molecular Gas	CrO	CrO

Table	Title	Conventional Formula	Filing Order
	Chromium Dioxide		
136	Condensed Phase	CrO_2	CrO_2
137	Ideal Molecular Gas	CrO_2	CrO_2
	Chromium Trioxide		
138	Condensed Phase	CrO_3	CrO_3
139	Ideal Molecular Gas	CrO_3	CrO_3
	Hafnium		
140	Reference State	Hf	Hf
141	Ideal Monatomic Gas	Hf	Hf
	Hafnium Nitride		
142	Condensed Phase	HfN	HfN
	Hafnium Monoxide		
143	Ideal Molecular Gas	HfO	HfO
	Hafnium Dioxide		
144	Condensed Phase	HfO_2	HfO_2
145	Ideal Molecular Gas	HfO_2	HfO_2
	Iridium		
146	Reference State	Ir	Ir
147	Ideal Monatomic Gas	Ir	Ir
	Iridium Monoxide		
148	Ideal Molecular Gas	IrO	IrO
	Magnesium		
149	Reference State	Mg	Mg
150	Ideal Monatomic Gas	Mg	Mg
	Magnesium Oxide		
151	Condensed Phase	MgO	MgO
152	Ideal Molecular Gas	MgO	MgO
	Magnesium Nitride		
153	Condensed Phase	Mg_3N_2	Mg_3N_2
	Manganese		
154	Reference State	Mn	Mn
155	Ideal Monatomic Gas	Mn	Mn

Table	Title	Conventional Formula	Filing Order
	Manganese Oxide		
156	Ideal Molecular Gas	MnO	MnO
	Molybdenum		
157	Reference State	Mo	Mo
158	Ideal Monatomic Gas	Mo	Mo
	Molybdenum Monoxide		
159	Ideal Molecular Gas	MoO	MoO
	Molybdenum Dioxide		
160	Condensed Phase	MoO_2	MoO_2
161	Ideal Molecular Gas	MoO_2	MoO_2
	Molybdenum Trioxide		
162	Condensed Phase	MoO_3	MoO_3
163	Ideal Molecular Gas	MoO_3	MoO_3
	Nitrogen		
164	Ideal Monatomic Gas	N	N
	Niobium Nitride		
165	Condensed Phase	NbN	NNb
	Diniobium Nitride		
166	Condensed Phase	Nb_2N	NNb_2
	Tantalum Nitride		
167	Condensed Phase	TaN	NTa
	Ditantalum Nitride		
168	Condensed Phase	Ta_2N	NTa_2
	Titanium Nitride		
169	Condensed Phase	TiN	NTi
	Zirconium Nitride		
170	Condensed Phase	ZrN	NZr
	Nitrogen		
171	Reference State	N_2	N_2

Table	Title	Conventional Formula	Filing Order
	Silicon Nitride		
172	Condensed Phase	Si_3N_4	N_4Si_3
	Niobium		
173	Reference State	Nb	Nb
174	Ideal Monatomic Gas	Nb	Nb
	Niobium Monoxide		
175	Condensed Phase	NbO	NbO
176	Ideal Molecular Gas	NbO	NbO
	Niobium Dioxide		
177	Condensed Phase	NbO_2	NbO_2
178	Ideal Molecular Gas	NbO_2	NbO_2
	Niobium Pentoxide		
179	Condensed Phase	Nb_2O_5	Nb_2O_5
	Oxygen		
180	Ideal Monatomic Gas	O	O
	Osmium Monoxide		
181	Ideal Molecular Gas	OsO	OOs
	Platinum Monoxide		
182	Ideal Molecular Gas	PtO	OPt
	Rhenium Monoxide		
183	Ideal Molecular Gas	ReO	ORe
	Rhodium Monoxide		
184	Ideal Molecular Gas	RhO	ORh
	Silicon Monoxide		
185	Ideal Molecular Gas	SiO	OSi
	Strontium Monoxide		
186	Condensed Phase	SrO	OSr
187	Ideal Molecular Gas	SrO	OSr
	Tantalum Monoxide		
188	Ideal Molecular Gas	TaO	OTa

Table	Title	Conventional Formula	Filing Order
	Technetium Monoxide		
189	Ideal Molecular Gas	TcO	OTc
	Thorium Monoxide		
190	Ideal Molecular Gas	ThO	OTh
	Titanium Monoxide		
191	Condensed Phase	TiO	OTi
192	Ideal Molecular Gas	TiO	OTi
	Uranium Monoxide		
193	Ideal Molecular Gas	UO	OU
	Tungsten Monoxide		
194	Ideal Molecular Gas	WO	OW
	Yttrium Monoxide		
195	Ideal Molecular Gas	YO	OY
	Zirconium Monoxide		
196	Ideal Molecular Gas	ZrO	OZr
	Oxygen		
197	Reference State	O_2	O_2
	Osmium Dioxide		
198	Ideal Molecular Gas	OsO_2	O_2Os
	Silicon Dioxide		
199	Condensed Phase	SiO_2	O_2Si
200	Ideal Molecular Gas	SiO_2	O_2Si
	Tantalum Dioxide		
201	Ideal Molecular Gas	TaO_2	O_2Ta
	Titanium Dioxide		
202	Condensed Phase	TiO_2	O_2Ti
203	Ideal Molecular Gas	TiO_2	O_2Ti
	Uranium Dioxide		
204	Condensed Phase	UO_2	O_2U
205	Ideal Molecular Gas	UO_2	O_2U

Table	Title	Conventional Formula	Filing Order
	Vanadium Dioxide		
206	Ideal Molecular Gas	VO_2	O_2V
	Tungsten Dioxide		
207	Condensed Phase	WO_2	O_2W
208	Ideal Molecular Gas	WO_2	O_2W
	Zirconium Dioxide		
209	Condensed Phase	ZrO_2	O_2Zr
210	Ideal Molecular Gas	ZrO_2	O_2Zr
	Osmium Trioxide		
211	Ideal Molecular Gas	OsO_3	O_3Os
	Titanium Sesquioxide		
212	Condensed Phase	Ti_2O_3	O_3Ti_2
	Tungsten Trioxide		
213	Condensed Phase	WO_3	O_3W
214	Ideal Molecular Gas	WO_3	O_3W
	Osmium Tetroxide		
215	Ideal Molecular Gas	OsO_4	O_4Os
	Tantalum Pentoxide		
216	Condensed Phase	Ta_2O_5	O_5Ta_2
	Trititanium Pentoxide		
217	Condensed Phase	Ti_3O_5	O_5Ti_3
	Rhenium Heptoxide		
218	Condensed Phase	Re_2O_7	O_7Re_2
	Osmium		
219	Reference State	Os	Os
220	Ideal Monatomic Gas	Os	Os
	Platinum		
221	Reference State	Pt	Pt
222	Ideal Monatomic Gas	Pt	Pt

Table	Title	Conventional Formula	Filing Order
	Rhenium		
223	Reference State	Re	Re
224	Ideal Monatomic Gas	Re	Re
	Rhodium		
225	Reference State	Rh	Rh
226	Ideal Monatomic Gas	Rh	Rh
	Scandium		
227	Reference State	Sc	Sc
228	Ideal Monatomic Gas	Sc	Sc
	Silicon		
229	Reference State	Si	Si
230	Ideal Monatomic Gas	Si	Si
	Strontium		
231	Reference State	Sr	Sr
232	Ideal Monatomic Gas	Sr	Sr
	Tantalum		
233	Reference State	Ta	Ta
234	Ideal Monatomic Gas	Ta	Ta
	Technetium		
235	Reference State	Tc	Tc
236	Ideal Monatomic Gas	Tc	Tc
	Thorium		
237	Reference State	Th	Th
238	Ideal Monatomic Gas	Th	Th
	Titanium		
239	Reference State	Ti	Ti
240	Ideal Monatomic Gas	Ti	Ti
	Uranium		
241	Reference State	U	U
242	Ideal Monatomic Gas	U	U
	Vanadium		
243	Reference State	V	V
244	Ideal Monatomic Gas	V	V

Table	Title	Conventional Formula	Filing Order
	Tungsten		
245	Reference State	W	W
246	Ideal Monatomic Gas	W	W
	Yttrium		
247	Reference State	Y	Y
248	Ideal Monatomic Gas	Y	Y
	Zirconium		
249	Reference State	Zr	Zr
250	Ideal Monatomic Gas	Zr	Zr

*At the bottom of the tables are listed the dates on which the tables have been completed and the initials of the scientist who prepared them. The same scientist has been responsible for the corresponding discussions which are given in volume 1 of this report.

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Griffel, M.	MG
Panish, M. B.	MBP
Schick, H. L.	HLS
Ward, C. H.	CHW

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VII
THERMODYNAMIC TABLES

TABLE 89

BORON — REFERENCE STATE — B

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p Solid B from 0° to 2450°K, Liquid B from 2450° to 3970°K, Gaseous B from 3970° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-0.290			
298.15	2.823	1.392	1.392	0.000			
300	2.845	1.409	1.389	0.006			
400	3.841	2.374	1.516	0.343			
500	4.498	3.307	1.783	0.762			
600	4.966	4.170	2.108	1.237			
700	5.333	4.964	2.461	1.752			
800	5.639	5.697	2.820	2.301			
900	5.902	6.377	3.178	2.879			
1000	6.130	7.011	3.530	3.481			
1100	6.329	7.605	3.874	4.104			
1200	6.502	8.163	4.208	4.746			
1300	6.652	8.689	4.532	5.403			
1400	6.783	9.187	4.847	6.075			
1500	6.897	9.659	5.153	6.759			
1600	6.996	10.107	5.448	7.454			
1700	7.083	10.534	5.735	8.158			
1800	7.160	10.941	6.013	8.870			
1900	7.228	11.330	6.282	9.590			
2000	7.288	11.703	6.545	10.316			
2100	7.341	12.059	6.798	11.047			
2200	7.388	12.402	7.045	11.784			
2300	7.430	12.731	7.285	12.525			
2400	7.468	13.048	7.519	13.269			
2450	7.485	13.222	7.654	13.642			
2450	7.500	15.522	7.654	19.277			
2500	7.500	15.673	7.812	19.652			
2600	7.500	15.967	8.120	20.402			
2700	7.500	16.250	8.416	21.152			
2800	7.500	16.523	8.7[illegible]1	21.902			
2900	7.500	16.786	8.975	22.652			
3000	7.500	17.041	9.240	23.402			
3100	7.500	17.287	9.496	24.152			
3200	7.500	17.525	9.743	24.902			
3300	7.500	17.756	9.982	25.652			
3400	7.500	17.979	10.214	26.402			
3500	7.500	18.197	10.439	27.152			
3600	7.500	18.408	10.658	27.902			
3700	7.500	18.614	10.870	28.652			
3800	7.500	18.814	11.077	29.402			
3900	7.500	19.009	11.277	30.152			
3969.96	7.500	19.142	11.415	30.676			
3969.96	4.981	49.513	11.415	151.248			
4000	4.982	49.551	11.702	151.397			
4100	4.985	49.674	12.626	151.896			
4200	4.988	49.794	13.510	152.394			
4300	4.993	49.912	14.356	152.893			
4400	4.997	50.027	15.165	153.393			
4500	5.002	50.139	15.941	153.893			
4600	5.008	50.249	16.685	154.393			
4700	5.015	50.357	17.401	154.894			
4800	5.022	50.463	18.089	155.396			
4900	5.030	50.566	18.750	155.899			
5000	5.038	50.668	19.388	156.402			
5100	5.048	50.768	20.002	156.906			
5200	5.058	50.866	20.595	157.412			
5300	5.069	50.962	21.166	157.918			
5400	5.081	51.057	21.719	158.426			
5500	5.093	51.151	22.254	158.934			
5600	5.107	51.242	22.770	159.444			
5700	5.121	51.333	23.271	159.956			
5800	5.136	51.422	23.755	160.468			
5900	5.152	51.510	24.225	160.983			
6000	5.168	51.597	24.681	161.499			

$0^\circ K$ to $2450^\circ K$	Crystal
$2450^\circ K$ to $3969.96^\circ K$	Liquid
$3969.96^\circ K$ to $6000^\circ K$	Ideal Monatomic Gas

$\Delta H^\circ_{f0} = 0$

$\Delta H^\circ_{f298.15} = 0$

$\Delta H^\circ_{s298.15} = 133.0$ Kcal gfw^{-1}

$S^\circ_{298.15} = 1.392$ cal $degK^{-1}$ gfw^{-1}

$T_m = 2450^\circ K$

$\Delta H_m = 5.635$ Kcal gfw^{-1}

$T_b = 3969.96^\circ K$

$\Delta H_v = 120.572$ Kcal gfw^{-1}

C°_p data from Wise *et al*[1].

Structure

Elemental boron has several crystalline modifications See earlier report[2] (p 1-76) for further details

Heat of Formation

Zero by definition

Heat Capacity and Entropy

Low temperature data from Johnston *et al*[3] and Wise *et al*[1]

Melting

Several values discussed in earlier report[2]

Heat of Sublimation

An average of several determination having scatter of about 8 Kcal See text for more details.

References

1. Wise, S., J. Margrave and R. L. Altman, J. Phys Chem. 64, 915 (1960).
2. Barriault, R. J. et al, Thermodynamics of Certain Refractory Compounds, Pt. I, Vol. 1, ASD TR-61-260 (May 1962).
3. Johnston, H. L., H. N Hersh and E. C. Kerr, J. Am. Chem. Soc. 73, 1112 (1951)

BORON (B) (REFERENCE STATE) GFW = 10.82

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal/gfw)	ΔH°_f (Kcal/gfw)	ΔF°_f (Kcal/gfw)	Log K_p
298.15	± 0.200	± 0.020	± 0.020	± 0.000			
1000	± 0.200	± 0.260	± 0.120	± 0.140			
2000	± 0.200	± 0.400	± 0.230	± 0.340			
2450	± 0.200	± 0.420	± 0.250	± 0.430			
2450	± 1.000	± 0.720	± 0.250	± 1.160			
3000	± 1.000	± 0.920	± 0.350	± 1.710			
3969.96	± 1.000	± 1.200	± 0.520	± 2.710			

TABLE 90

BORON | IDEAL MONATOMIC GAS | B

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid B from 0° to 2450°K, Liquid B from 2450° to 3970°K, Gaseous B from 3970° to 6000°K.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.511	131.779	131.779	INFINITE
298.15	4.971	36.649	36.649	0.000	133.000	122.489	-89.782
300	4.971	36.680	36.650	0.009	133.003	122.422	-89.180
400	4.970	38.110	36.845	0.506	133.163	118.869	-64.943
500	4.969	39.218	37.212	1.003	133.241	115.286	-50.389
600	4.969	40.124	37.624	1.500	133.263	111.691	-40.681
700	4.969	40.890	38.037	1.997	133.245	108.097	-33.747
800	4.968	41.554	38.436	2.494	133.193	104.508	-28.548
900	4.968	42.139	38.815	2.991	133.112	100.927	-24.507
1000	4.968	42.662	39.175	3.487	133.006	97.355	-21.275
1100	4.968	43.136	39.514	3.984	132.880	93.796	-18.634
1200	4.968	43.568	39.833	4.481	132.735	90.250	-16.435
1300	4.968	43.966	40.136	4.978	132.575	86.715	-14.577
1400	4.968	44.[illegible]	40.423	5.475	132.400	83.194	-12.986
1500	4.968	44.[illegible]77	40.675	5.972	132.213	79.687	-11.609
1600	4.968	44.998	40.955	6.468	132.014	76.189	-10.4[illegible]6
1700	4.968	45.299	41.2[illegible]2	6.965	131.807	72.707	-9.346
1800	4.968	45.583	41.437	7.462	131.592	69.237	-8.406
1900	4.968	45.851	41.667	7.959	131.369	65.778	-7.565
2000	4.968	46.106	41.878	8.446	131.140	62.334	-6.811
2100	4.968	46.34[illegible]	42.086	8.952	130.905	58.896	-6.129
2200	4.968	46.580	42.285	9.449	130.665	55.472	-5.510
2300	4.968	46.801	42.476	9.946	130.421	52.061	-4.946
2400	4.968	47.012	42.660	10.443	130.174	48.662	-4.431
2450	4.968	47.114	42.750	10.691	130.049	47.015	-4.193
2450	4.968	47.114	42.750	10.691	124.414	47.015	-4.193
2500	4.968	47.215	42.839	10.940	124.288	45.433	-3.971
2600	4.968	47.410	43.011	11.437	124.035	42.284	-3.554
2700	4.968	47.597	43.177	11.933	123.781	39.146	-3.168
2800	4.968	47.778	43.338	12.430	123.528	36.017	-2.811
2900	4.969	47.952	43.494	12.927	123.275	32.895	-2.478
3000	4.969	48.121	43.646	13.424	123.022	29.782	-2.169
3100	4.969	48.284	43.793	13.921	122.769	26.680	-1.880
3200	4.970	48.441	43.935	14.418	122.516	23.586	-1.610
3300	4.970	48.594	44.074	14.915	[illegible].269	20.497	-1.357
3400	4.971	48.743	44.212	15.412	1[illegible]010	17.414	-1.119
3500	4.972	48.887	44.341	15.909	12[illegible]757	14.343	-0.895
3600	4.973	49.027	44.469	16.406	121.504	11.281	-0.684
3700	4.975	49.163	44.[illegible]94	16.904	121.252	8.222	-0.485
3800	4.977	49.2[illegible]6	44.716	17.401	120.999	5.172	-0.297
3900	4.979	49.425	44.835	17.899	120.747	2.124	-0.119
3969.96	4.981	49.513	44.916	18.247	120.571	0.000	0.000
3969.96	4.981	49.513	44.916	18.247			
4000	4.982	49.551	44.951	18.397			
4100	4.985	49.674	45.066	18.896			
4200	4.988	49.794	45.176	19.394			
4300	4.993	49.912	45.285	19.893			
4400	4.997	50.0[illegible]7	45.392	20.393			
4500	5.002	50.139	45.4[illegible]6	20.893			
4600	5.008	50.249	45.598	21.393			
4700	5.015	50.357	45.698	21.894			
4800	5.022	50.463	45.79[illegible]	22.396			
4900	5.030	50.566	45.8[illegible]	22.899			
5000	5.038	50.668	45.987	23.402			
5100	5.048	50.768	46.080	23.906			
5200	5.058	50.866	46.171	24.412			
5300	5.069	50.962	46.260	24.918			
5400	5.081	51.057	46.348	25.426			
5500	5.093	51.151	46.435	25.934			
5600	5.107	51.242	46.519	26.444			
5700	5.12[illegible]	51.333	46.603	26.956			
5800	5.135	51.422	46.686	27.468			
5900	5.152	51.510	46.767	27.983			
6000	5.168	51.597	46.847	28.499			

15 March 1963 | HLS

ΔH^{o}_{f0} = 131.779 Kcal gfw^{-1}

Ground State Configuration $^{2}P_{\frac{1}{2}}$

$H^{o}_{298.15}-H^{o}_{0}$ = 1.511 Kcal gfw^{-1}

$\Delta H^{o}_{f298.15}$ = 133.0 Kcal gfw^{-1}

$S^{o}_{298.15}$ = 36.649 cal degK^{-1} gfw^{-1}

Electronic Levels and Multiplicities

Data from earlier report.[1]

Heat of Formation

An average of several determinations having scatter of about 8 Kcal. See earlier report[1] and volume 1, this report for more details.

Heat Capacity and Entropy

From earlier report.[1]

Reference

1. Barriault, R. J. et al, Thermodynamics of Certain Refractory Compounds, Pt. I, Vol. 1, ASD TR-61-260 (May 1962).

BORON, MONATOMIC (B) (IDEAL GAS) gfw = 10.82

SUMMARY OF UNCERTAINTY ESTIMATE

T °K	Cp	S	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
298.15	± 0.001	± 0.001	± 0.001	± 0.000	±4.000	±4.000	± 2.910
1000	± 0.001	± 0.001	± 0.001	± 0.001			
2000	± 0.001	± 0.001	± 0.001	± 0.002			
2450	± 0.001	± 0.001	± 0.001	± 0.002			
2450	± 0.001	± 0.001	± 0.001	± 0.002			
3000	± 0.001	± 0.001	± 0.001	± 0.003			
3969.96	± 0.001	± 0.001	± 0.001	± 0.004			

TABLE 91

HAFNIUM DIBORIDE — CONDENSED PHASE — B_2Hf

Reference State for Calculating $\Delta H_f°$, $\Delta F_f°$, and Log K_f: Solid Hf from 0° to 2495°K, Liquid Hf from 2495° to 4985°K, Gaseous Hf from 4985° to 6000°K, Solid B from 0° to 2450°K, Liquid B from 2450° to 3970°K, Gaseous B from 3970° to 6000°K, Solid HfB_2 from 0° to 3523°K, Liquid HfB_2 from 3523° to 6000°K.

T, °K	$C_p°$ (cal/°K gfw)	$S_T°$ (cal/°K gfw)	$-(F_T°-H_{298}°)/T$ (cal/°K gfw)	$H_T°-H_{298}°$ (Kcal/gfw)	$\Delta H_f°$ (Kcal/gfw)	$\Delta F_f°$ (Kcal/gfw)	Log K_f
0	0.000	0.000	INFINITE	-1.706	-79.691	-79.691	INFINITE
298.15	12.000	11.068	11.068	0.000	-80.000	-79.277	58.109
300	12.080	11.142	11.068	0.022	-80.002	-79.274	57.748
400	14.941	15.065	11.584	1.392	-79.970	-79.035	43.181
500	16.365	18.567	12.638	2.965	-79.937	-78.806	34.444
600	17.224	21.632	13.887	4.647	-79.930	-78.585	28.623
700	17.816	24.334	15.190	6.401	-79.948	-78.358	24.463
800	18.266	26.744	16.487	8.206	-79.999	-78.127	21.342
900	18.633	28.917	17.749	10.051	-80.086	-77.888	18.913
1000	18.949	30.897	18.966	11.931	-80.203	-77.637	16.967
1100	19.231	32.716	20.135	13.840	-80.349	-77.374	15.372
1200	19.490	34.401	21.254	15.776	-80.523	-77.096	14.040
1300	19.734	35.971	22.326	17.737	-80.721	-76.803	12.911
1400	19.965	37.442	23.354	19.722	-80.940	-76.494	11.941
1500	20.188	38.827	24.340	21.730	-81.177	-76.166	11.097
1600	20.404	40.136	25.287	23.760	-81.432	-75.827	10.357
1700	20.616	41.380	26.197	25.811	-81.700	-75.466	9.701
1800	20.823	42.564	27.074	27.883	-81.980	-75.095	9.117
1900	21.027	43.695	27.919	29.975	-82.274	-74.705	8.593
2000	21.228	44.779	28.735	32.088	-82.575	-74.292	8.118
2033	21.294	45.127	28.998	32.790	-82.676	-74.153	7.971
2033	21.294	45.127	28.998	32.790	-84.326	-74.153	7.971
2100	21.426	45.820	29.524	34.221	-84.533	-73.822	7.682
2200	21.626	46.821	30.288	36.374	-84.850	-73.305	7.282
2300	21.822	47.787	31.028	38.546	-85.173	-72.773	6.915
2400	22.017	48.720	31.745	40.738	-85.499	-72.224	6.577
2450	22.114	49.175	32.096	41.841	-85.644	-71.859	6.410
2450	22.114	49.175	32.096	41.841	-96.914	-71.859	6.410
2495	22.201	49.578	32.408	42.838	-97.086	-71.387	6.253
2495	22.201	49.578	32.408	42.838	-102.325	-71.387	6.253
2500	22.211	49.622	32.442	42.949	-102.328	-71.323	6.235
2600	22.405	50.497	33.120	45.180	-102.397	-70.084	5.891
2700	22.597	51.346	33.780	47.430	-102.447	-68.841	5.572
2800	22.789	52.172	34.422	49.700	-102.477	-67.593	5.276
2900	22.981	52.975	35.046	51.988	-102.489	-66.350	5.000
3000	23.172	53.757	35.658	54.296	-102.481	-65.099	4.742
3100	23.362	54.520	36.255	56.623	-102.454	-63.852	4.501
3200	23.553	55.265	36.837	58.968	-102.409	-62.608	4.276
3300	23.743	55.992	37.40	61.333	-102.344	-61.368	4.064
3400	23.932	56.704	37.964	63.717	-102.260	-60.127	3.865
3500	24.122	57.400	38.519	66.120	102.157	-58.868	3.677
3523	24.165	57.559	38.633	66.675	-102.130	-58.601	3.635
3523	24.165	63.235	38.633	86.675	-82.130	-58.601	3.635
3600	24.165	63.758	39.165	88.536	-82.041	-58.087	3.526
3700	24.165	64.420	39.838	90.952	-81.925	-57.423	3.392
3800	24.165	65.065	40.494	93.369	-81.808	-56.759	3.264
3900	24.165	65.692	41.132	95.785	-81.692	-56.109	3.144
3969.96	24.165	66.122	41.567	97.476	-81.609	-55.648	3.063
3969.96	24.165	66.122	41.567	97.476	-322.753	-55.648	3.063
4000	24.165	66.304	41.754	98.201	-322.565	-53.624	2.930
4100	24.165	66.901	42.363	100.618	-321.947	-46.913	2.501
4200	24.165	67.483	42.951	103.035	-321.326	-40.205	2.092
4300	24.165	68.052	43.524	105.451	-320.705	-33.513	1.703
4400	24.165	68.607	44.081	107.868	-320.091	-26.844	1.333
4500	24.165	69.150	44.643	110.284	-319.475	-20.186	0.980
4600	24.165	69.681	45.181	112.701	-318.858	-13.546	0.644
4700	24.165	70.201	45.706	115.117	-318.244	-6.910	0.321
4800	24.165	70.710	46.224	117.534	-317.631	-0.291	0.013
4900	24.165	71.208	46.728	119.950	-317.021	6.309	-0.281
4985.40	24.165	71.625	47.151	122.014	-316.500	11.941	-0.523
4985.40	24.165	71.625	47.151	122.014	-449.796	11.941	-0.523
5000	24.165	71.696	47.223	122.367	-449.719	13.295	-0.581
5100	24.165	72.175	47.708	124.783	-449.205	22.546	-0.966
5200	24.165	72.644	48.183	127.200	-448.704	31.795	-1.336
5300	24.165	73.104	48.648	129.616	-448.212	41.020	-1.691
5400	24.165	73.556	49.106	132.033	-447.732	50.248	-2.034
5500	24.165	73.999	49.554	134.449	-447.261	59.474	-2.363
5600	24.165	74.435	49.995	136.866	-446.802	68.674	-2.680
5700	24.165	74.863	50.427	139.282	-446.356	77.884	-2.986
5800	24.165	75.283	50.852	141.699	-445.917	87.069	-3.281
5900	24.165	75.696	51.270	144.115	-445.492	96.262	-3.566
6000	24.165	76.102	51.680	146.532	-445.076	105.448	-3.841

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HAFNIUM DIBORIDE (HfB_2) (CONDENSED PHASE) gfw = 200.14

$\Delta H^{\circ}_{f298.15} = -80.0$ kcal gfw^{-1}

$S^{\circ}_{298.15} = 11.068$ cal deg K^{-1} gfw^{-1}

$T_m = 3523^{\circ}K$

$\Delta H_m = 20.0$ kcal gfw^{-1}

$H^{\circ}_{298.15} - H^{\circ}_0 = 1.706$ kcal gfw^{-1}

$C^{\circ}_p = 17.632 + 1.867 \times 10^{-3}\ T - 5.501 \times 10^{5}\ T^{-2}$ cal deg K^{-1} gfw^{-1}

$298.15^{\circ}K \leq T \leq 2813^{\circ}K$

Structure

Hexagonal type (isotypic with ZrB_2). Narrow range of homogeneity.

Heat of Formation

Value is based on tensimetric data of Paderno *et al*,[1] vaporization data of Krupka;[2] and nitrogen equilibria of Rudy and Benesovsky.[3]

Heat Capacity and Entropy

Low-temperature data have been estimated. High-temperature data of Mezaki *et al*[4] and Pears *et al*[5] have been recalculated. Heat-capacity equation has been extrapolated to melting point. Data for liquid are estimated.

Melting and Vaporization

Heat of fusion is estimated.

References

1. Paderno, Y. *et al*, Tsvetnye Metally 11, 48-50 (1959).
2. Krupka, M., LA-2611 (1962).
3. Rudy, E. and F. Benesovsky, Monatsh. Chem. 92, 427 (1961).
4. Mezaki, R. *et al*, In: Thermodynamics of Nuclear Materials, Internatl. At. Energy Agency, Vienna (1962).
5. Pears, C. D. *et al*, ASD TDR 62-765 (January 1963).

TABLE 92

NIOBIUM DIBORIDE CONDENSED PHASE B_2Nb

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Nb from 0° to 2741 °K, Liquid Nb from 2741° to 5032 °K, Gaseous Nb from 5032° to 6000 °K, Solid B from 0° to 2450 °K, Liquid B from 2450° to 3970 °K, Gaseous B from 3970° to 6000 °K, Solid NbB_2 from 0° to 3273 °K, Liquid NbB_2 from 3273° to 6000 °K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (kcal/gfw)	ΔH_f° (kcal/gfw)	ΔF_f° (kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.630	-41.686	-41.686	INFINITE
298.15	11.500	8.960	8.960	0.000	-41.900	-41.058	30.095
300	11.557	9.031	8.960	0.021	-41.902	-41.055	29.907
400	13.797	12.695	9.445	1.300	-41.897	-40.771	22.275
500	15.207	15.934	10.425	2.754	-41.890	-40.489	17.697
600	16.291	18.805	11.587	4.331	-41.882	-40.212	14.647
700	17.220	21.388	12.806	6.007	-41.864	-39.934	12.467
800	18.067	23.743	14.028	7.772	-41.835	-39.661	10.834
900	18.866	25.918	15.230	9.619	-41.792	-39.392	9.565
1000	19.635	27.945	16.401	11.544	-41.728	-39.128	8.551
1100	20.385	29.852	17.538	13.546	-41.639	-38.871	7.723
1200	21.122	31.657	18.640	15.621	-41.524	-38.625	7.034
1300	21.550	33.365	19.708	17.755	-41.390	-38.391	6.454
1400	21.979	34.978	20.741	19.931	-41.254	-38.163	5.957
1500	22.407	36.509	21.742	22.150	-41.108	-37.946	5.528
1600	22.835	37.969	22.711	24.412	-40.951	-37.743	5.155
1700	23.263	39.366	23.650	26.717	-40.778	-37.548	4.827
1800	23.692	40.708	24.560	29.065	-40.588	-37.362	4.536
1900	24.120	42.000	25.444	31.456	-40.381	-37.190	4.278
2000	24.548	43.248	26.304	33.889	-40.153	-37.024	4.046
2100	24.976	44.456	27.139	36.365	-39.902	-36.877	3.838
2200	25.405	45.628	27.953	38.884	-39.629	-36.741	3.650
2300	25.833	46.767	28.747	41.446	-39.331	-36.617	3.479
2400	26.261	47.875	29.521	44.051	-39.006	-36.505	3.324
2450	26.475	48.419	29.901	45.369	-38.833	-36.353	3.243
2450	26.475	48.419	29.901	45.369	-50.103	-36.353	3.243
2500	26.689	48.956	30.276	46.699	-49.925	-36.075	3.154
2600	27.118	50.011	31.015	49.389	-49.546	-35.530	2.986
2700	27.546	51.042	31.738	52.122	-49.133	-34.999	2.833
2741	27.722	51.459	32.030	53.255	-48.953	-34.787	2.774
2741	27.722	51.459	32.030	53.255	-55.353	-34.787	2.774
2800	27.974	52.052	32.446	54.898	-55.068	-34.346	2.681
2900	28.403	53.041	33.139	57.717	-54.549	-33.615	2.533
3000	28.831	54.011	33.818	60.579	-53.987	-32.900	2.397
3100	29.259	54.964	34.485	63.483	-53.383	-32.203	2.270
3200	29.687	55.899	35.140	66.430	-52.736	-31.535	2.154
3273	30.000	56.572	35.610	68.609	-52.235	-31.057	2.074
3273	30.000	62.683	35.610	88.609	-32.235	-31.057	2.074
3300	30.000	62.929	35.833	89.419	-32.047	-31.050	2.056
3400	30.000	63.825	36.643	92.419	-31.347	-31.027	1.994
3500	30.000	64.695	37.432	95.419	-30.647	-31.029	1.937
3600	30.000	65.540	38.201	98.419	-29.947	-31.046	1.885
3700	30.000	66.362	38.951	101.419	-29.247	-31.089	1.836
3800	30.000	67.162	39.683	104.419	-28.547	-31.142	1.791
3900	30.000	67.941	40.398	107.419	-27.847	-31.230	1.750
3969.96	30.000	68.474	40.888	109.518	-27.356	-31.288	1.722
3969.96	30.000	68.474	40.888	109.518	-268.500	-31.288	1.722
4000	30.000	68.701	41.096	110.419	-268.137	-29.488	1.611
4100	30.000	69.441	41.778	113.419	-266.935	-23.540	1.255
4200	30.000	70.164	42.446	116.419	-265.731	-17.620	0.917
4300	30.000	70.870	43.098	119.419	-264.529	-11.714	0.595
4400	30.000	71.560	43.73[illegible]	122.419	-263.329	-5.851	0.291
4500	30.000	72.234	44.36	125.419	-262.129	-0.014	0.001
4600	30.000	72.893	44.976	128.419	-260.929	5.793	-0.275
4700	30.000	73.539	45.577	131.419	-259.731	11.581	-0.539
4800	30.000	74.170	46.166	134.419	-258.535	17.346	-0.790
4900	30.000	74.789	46.744	137.419	-257.341	23.074	-1.029
5000	30.000	75.395	47.311	140.419	-256.147	28.790	-1.258
5031.58	30.000	75.584	47.488	141.366	-255.771	30.520	-1.326
5031.58	30.000	75.584	47.488	141.366	-418.344	30.520	-1.326
5100	30.000	75.989	47.858	143.419	-417.570	36.620	-1.569
5200	30.000	76.572	48.414	146.419	-416.449	45.522	-1.913
5300	30.000	77.143	48.951	149.419	-415.333	54.380	-2.242
5400	30.000	77.704	49.478	152.419	-414.226	63.238	-2.559
5500	30.000	78.254	49.996	155.419	-413.125	72.076	-2.864
5600	30.000	78.795	50.506	158.419	-412.032	80.874	-3.156
5700	30.000	79.326	51.007	161.419	-410.948	89.673	-3.438
5800	30.000	79.848	51.492	164.419	-409.868	98.448	-3.709
5900	30.000	80.360	51.984	167.419	-408.798	107.205	-3.971
6000	30.000	80.865	52.461	170.419	-407.734	115.948	-4.223

15 September 1963 HLS

NIOBIUM DIBORIDE (NbB_2) (CONDENSED PHASE) gfw = 114.55

$\Delta H^\circ_{f\,298.15} = -41.9$ kcal gfw^{-1} $S^\circ_{298.15} = 8.96$ cal $degK^{-1} gfw^{-1}$

$T_m = 3273°K$ $\Delta H_m = 20.0$ kcal gfw^{-1}

$H^\circ_{298.15} - H^\circ_0 = 1.630$ kcal gfw^{-1}

$C^\circ_p = 13.004 + 6.9491 \times 10^{-3} T - 3.1784 \times 10^5 T^{-2}$ $298.15°K \leq T \leq 1200°K$

$C^\circ_p = 15.983 + 0.0042826\ T$ cal deg K^{-1} gfw^{-1} $1200°K \leq T \leq 3273°K$

$C^\circ_p = 30.0$ cal deg K^{-1} gfw^{-1} $3773°K \leq T \leq 6000°K$

Structure

NbB_2 has a hexagonal structure

Heat of Formation

Based on unpublished heat of combustion studies by Huber [1]

Heat Capacity and Entropy

Low temperature data was obtained by Westrum[2] for $NbB_{1.975}$. A minor correction was made to the stoichiometric composition. Data from 298.15 to 1200°K were analyzed by Shomate method using Tilleux's[3] enthalpy values Data above 1200°K was estimated.

Melting and Vaporization

Melting point was tabulated by Nowotny et al[4]. Heat of melting was estimated

References

1. Huber, E., Jr., Private Communication, April 1, 1963.
2. Westrum E. F., In: Kaufman, L. and E. Clougherty, Investigation of Boride Compounds for Very High Temperature Applications, Man Labs Semi-Annual Report No. 2, Contract AF33(657)-8635 (April 1963); See Also Final Report, Same Contract, RTD-TDR-63-4096, Part I (December 1963).
3. Tilleux, E. W., M. S. Thesis, U. of Wisconsin, January 1963
4. Nowotny, H. et al., Z. Metallkunde 50, 417 (1959).

NIØBIUM DIBØRIDE (NbB_2) (CØNDENSED PHASE) GFW = 114.55

SUMMARY ØF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal gfw)	ΔH_f (Kcal gfw)	ΔF_f (Kcal gfw)	Log K_p
298.15	±0.500	±0.100	±0.100	±0.000			
1000	±0.500	±0.705	±0.354	±0.351			
1500	±0.500	±0.908	±0.507	±0.601			
1500	±2.000	±0.908	±0.507	±0.601			
2000	±2.000	±1.483	±0.683	±1.601			
3000	±2.000	±2.294	±1.094	±3.601			
3273	±2.000	±2.468	±1.201	±4.147			
3273	±3.000	±3.996	±1.201	±9.147			
4000	±3.000	±4.598	±1.766	±11.328			
5000	±3.000	±5.267	±2.402	±14.328			
6000	±3.000	±5.814	±2.926	±17.328			

TABLE 93

TANTALUM DIBORIDE — CONDENSED PHASE — B_2Ta

Reference State for Calculating ΔH_f°, ΔF_f° and Log K_p: Solid Ta from 0° to 3270°K, Liquid Ta from 3270° to 5706°K, Gaseous Ta from 5706° to 6000°K, Solid B from 0° to 2450°K, Liquid B from 2450° to 3970°K, Gaseous B from 3970° to 6000°K, Solid TaB_2 from 0° to 3373°K, Liquid TaB_2 from 3373° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.665	-49.700	-49.700	INFINITE
298.15	11.500	10.603	10.603	0.000	-50.000	-49.374	36.190
300	11.559	10.674	10.603	0.021	-50.002	-49.371	35.965
400	13.759	14.337	11.088	1.300	-50.016	-49.158	26.857
500	15.019	17.553	12.066	2.743	-50.044	-48.939	21.390
600	15.908	20.373	13.221	4.291	-50.088	-48.717	17.744
700	16.623	22.881	14.425	5.919	-50.139	-48.483	15.136
800	17.245	25.142	15.625	7.613	-50.199	-48.242	13.179
900	17.813	27.206	16.799	9.366	-50.262	-47.994	11.654
1000	18.347	29.111	17.936	11.174	-50.324	-47.739	10.433
1100	18.859	30.883	19.034	13.035	-50.378	-47.478	9.432
1200	19.356	32.546	20.091	14.946	-50.426	-47.212	8.598
1300	19.842	34.114	21.110	16.906	-50.459	-46.945	7.892
1400	20.321	35.602	22.092	18.914	-50.480	-46.672	7.286
1500	20.794	37.020	23.041	20.970	-50.485	-46.398	6.760
1600	21.263	38.377	23.9[illegible]7	23.072	-50.472	-46.128	6.300
1700	21.728	39.680	24.844	25.222	-50.436	-45.857	5.895
1800	22.191	40.935	25.703	27.418	-50.379	-45.588	5.535
1900	22.652	42.148	26.537	29.660	-50.300	-45.328	5.214
2000	23.111	43.321	27.347	31.948	-50.199	-45.064	4.924
2100	23.569	44.460	28.135	34.282	-50.073	-44.815	4.664
2200	24.026	45.567	28.902	36.662	-49.925	-44.566	4.427
2300	24.482	46.645	29.650	39.088	-49.755	-44.326	4.212
2400	24.937	47.697	30.380	41.559	-49.562	-44.094	4.015
2450	25.164	48.213	30.739	42.811	-49.460	-43.880	3.914
2450	25.164	48.213	30.737	42.811	-60.730	-43.880	3.914
2500	25.391	48.724	31.094	44.075	-60.626	-43.542	3.806
2600	25.845	49.728	31.791	46.637	-60.397	-42.863	3.603
2700	26.298	50.712	32.474	49.244	-60.157	-42.192	3.415
2800	26.751	51.677	33.142	51.896	-59.912	-41.530	3.241
2900	27.204	52.624	33.798	54.594	-59.672	-40.880	3.081
3000	27.656	53.553	34.441	57.337	-59.449	-40.235	2.931
3100	28.108	54.468	35.072	60.125	-59.250	-39.593	2.791
3200	28.560	55.367	35.693	62.959	-59.082	-38.966	2.661
3270	28.876	55.969	36.120	64.969	58.987	-38.526	2.575
3270	28.876	55.989	36.120	64.969	55.687	-38.526	2.575
3300	29.011	56.25[illegible]	36.30[illegible]	65.837	- 5.524	-38.278	2.535
3373	29.341	56.891	36.741	67.967	55.108	-37.682	2.441
3373	30.000	62.821	36.741	87.967	-45.108	-37.682	2.441
3400	30.000	63.060	36.949	88.777	-44.934	-37.624	2.418
3500	30.000	63.930	37.707	91.777	-44.284	-37.414	2.336
3600	30.000	64.775	38.448	94.777	-43.634	-37.227	2.260
3700	30.000	65.597	39.170	97.777	-42.984	-37.057	2.189
3800	30.000	66.397	39.876	100.777	-42.334	-36.901	2.122
3900	30.000	67.176	40.566	103.777	-41.684	-36.775	2.061
3969.96	30.000	67.709	41.040	105.876	-41.228	-36.689	2.020
3969.96	30.000	67.709	41.040	105.876	82.372	-36.689	2.020
4000	30.000	67.935	41.241	106.777	-282.024	-34.824	1.903
4100	30.000	68.676	41.901	109.777	-280.872	-28.664	1.526
4200	30.000	69.399	42.547	112.777	-279.718	-22.519	1.172
4300	30.000	70.105	43.180	115.777	-278.566	-16.404	0.834
4400	30.000	70.795	43.800	118.777	-277.416	-10.325	0.513
4500	30.000	71.469	44.[illegible]7	121.777	-276.266	-4.266	0.207
4600	30.000	72.128	45.003	124.777	-275.116	1.759	-0.084
4700	30.000	72.773	45.587	127.777	-273.968	7.772	-0.361
4800	30.000	73.405	46.160	130.777	-272.822	13.758	-0.626
4900	30.000	74.024	46.722	133.777	-271.678	19.707	-0.879
5000	30.000	74.630	47.274	136.777	-270.534	25.650	-1.121
5100	30.000	75.224	47.817	139.777	-269.392	31.559	-1.352
5200	30.000	75.806	48.349	142.777	-268.254	37.454	-1.574
5300	30.000	76.378	48.873	145.777	-267.116	43.306	-1.786
5400	30.000	76.939	49.387	148.777	-265.982	49.160	-1.990
5500	30.000	77.489	49.893	151.777	-264.848	54.995	-2.185
5600	30.000	78.030	50.391	154.777	-263.718	60.790	-2.372
5700	30.000	78.561	50.880	157.777	-262.592	66.582	-2.553
5706.65	30.000	78.596	50.913	157.977	-262.516	66.963	-2.564
5706.65	30.000	78.596	50.913	157.977	-443.739	66.963	-2.564
5800	30.000	79.082	51.362	160.777	-442.842	75.303	-2.837
5900	30.000	79.595	51.836	163.777	-441.890	84.231	-3.120
6000	30.000	80.099	52.303	166.777	-440.943	93.148	-3.393

31 December 1963 HLS

TANTALUM DIBORIDE (TaB_2) **(CONDENSED PHASE)** gfw = 202.59

$\Delta H^o_{f298.15}$ = -50.0 kcal gfw^{-1}

$S^o_{298.15}$ = 10.603 cal deg K^{-1} gfw^{-1}

T_m = 3373°K

ΔH_m = 20.0 kcal gfw^{-1}

$H^o_{298.15} - H^o_0$ = 1.665 kcal gfw^{-1}

$C^o_p = 14.212 + 0.44947 \times 10^{-2}T - 0\ 36017 \times 10^6 T^{-2}$ cal deg K^{-1}gfw^{-1} 298 15°K ≤ T ≤ 3373°K

C^o_p = 30.0 cal deg K^{-1} gfw^{-1} 3373°K ≤ T ≤ 6000°K

Structure

TaB_2 has an hexagonal structure of the AlB_2 (C32) type. It has a wide homogeneity range.

Heat of Formation

Rough estimate used.

Heat Capacity and Entropy

Low-temperature data estimated See text for details. High-temperature data by Mezaki[1] and Neel *et al*[2] analyzed in this work and extrapolated to melting point.

Melting and Vaporization

Heat of fusion estimated

References

1. Mezaki, R., M S. Thesis, U. Wisc. (1961).

2. Neel, D. S. *et al*, WADD TR 60-924 (1962)

TANTALUM DI30RIDE (TaB_2) (CØNDENSED PHASE) GFW = 202.59

SUMMARY ØF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S_T (cal/°K gfw)	$-(F^o_T - H^o_{298})/T$ (cal/°K gfw)	$H_T - H_{298}$ (kcal gfw)	ΔH_f (kcal gfw)	ΔF_f (kcal gfw)	Log K_p
298.15	± 1.000	± 1.000	± 1.000	± 0.000	± 10.000		
1000	± 1.000	± 2.210	± 1.508	± 0.702			
2000	± 1.000	± 2.903	± 2.052	± 1.702			
2450	± 1.000	± 3.106	± 2.228	± 2.152			
2450	± 2.000	± 3.106	± 2.228	± 2.152			
3000	± 2.000	± 3.511	± 2.427	± 3.252			
3373	± 2.000	± 3.746	± 2.560	± 3.998			
3373	± 4.000	± 5.228	± 2.560	± 8.998			
4000	± 4.000	± 5.910	± 3.034	± 11.506			
5000	± 4.000	± 6.803	± 3.701	± 15.506			
6000	± 4.000	± 7.532	± 4.281	± 19.506			

TABLE 94

TITANIUM DIBORIDE CONDENSED PHASE B_2Ti

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p Solid Ti from 0° to 1950°K, Liquid Ti from 1950° to 3550°K, Gaseous Ti from 3550° to 6000°K, Solid B from 0° to 2450°K, Liquid B from 2450° to 3970°K, Gaseous B from 3970° to 6000°K, Solid TiB_2 from 0° to 3193°K, Liquid TiB_2 from 3193° to 6000°K.

T, °K	cal/°K gfw C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	Kcal/gfw $H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.381	-66.501	-66.501	INFINITE
298.15	10.503	6.700	6.700	0.000	-66.850	-65.832	48.254
300	10.579	6.765	6.700	0.020	-66.853	-65.828	47.953
400	13.373	10.241	7.155	1.234	-66.933	-65.471	35.770
500	14.868	13.400	8.094	2.653	-67.001	-65.096	28.452
600	15.851	16.202	9.217	4.191	-67.086	-64.711	23.570
700	16.592	18.704	10.397	5.815	-67.186	-64.306	20.076
800	17.204	20.960	11.578	7.506	-67.303	-63.887	17.452
900	17.741	23.018	12.737	9.253	-67.437	-63.452	15.407
1000	18.232	24.913	13.861	11.052	-67.582	-63.001	13.768
1100	18.692	26.673	14.947	12.899	-67.735	-62.536	12.424
1155	18.936	27.591	15.527	13.933	-67.823	-62.273	11.783
1155	18.936	27.591	15.527	13.933	-68.773	-62.273	11.783
1200	19.132	28.318	15.993	14.790	-68.844	-62.019	11.295
1300	19.557	29.866	17.001	16.725	-69.001	-61.446	10.329
1400	19.972	31.331	17.973	18.701	-69.159	-60.858	9.500
1500	20.379	32.723	18.910	20.719	-69.309	-60.257	8.779
1600	20.779	34.051	19.815	22.777	-69.452	-59.652	8.148
1700	21.176	35.322	20.690	24.874	-69.584	-59.033	7.589
1800	21.568	36.544	21.537	27.012	-69.701	-58.410	7.092
1900	21.958	37.720	22.358	29.188	-69.806	-57.781	6.646
1950	22.152	38.293	22.760	30.291	-69.851	-57.465	6.440
1950	22.152	38.293	22.760	30.291	-73.551	-57.465	6.440
2000	22.345	38.857	23.155	31.403	-73.568	-57.048	6.234
2100	22.731	39.956	23.929	33.657	-73.576	-56.226	5.851
2200	23.115	41.023	24.682	35.949	-73.558	-55.401	5.503
2300	23.498	42.058	25.415	38.280	-73.509	-54.577	5.186
2400	23.880	43.067	26.130	40.649	-73.428	-53.753	4.895
2450	24.070	43.561	26.480	41.848	-73.375	-53.240	4.749
2450	24.070	43.561	26.480	41.848	-84.645	-53.240	4.749
2500	24.260	44.049	26.827	43.056	-84.587	-52.607	4.599
2600	24.640	45.008	27.508	45.501	-84.442	-51.331	4.315
2700	25.020	45.945	28.173	47.984	-84.259	-50.059	4.052
2800	25.398	46.862	28.824	50.505	-84.038	-48.793	3.808
2900	25.777	47.760	29.462	53.064	-83.779	-47.542	3.583
3000	26.155	48.640	30.087	55.660	-83.483	-46.297	3.373
3100	26.532	49.504	[illegible]	58.295	[illegible]	-45.060	3.177
3193	26.883	50.293	31.258	60.778	-92.803	-43.924	3.006
3193	25.000	57.193	31.258	82.810	[illegible]	-43.924	3.006
3200	25.000	57.248	31.315	82.985	-60.758	-43.887	2.997
3300	25.000	58.017	32.113	85.485	-60.558	-43.364	2.872
3400	25.000	58.764	32.886	87.985	-60.358	-42.846	2.754
3500	25.000	59.488	33.635	90.485	-60.158	-42.332	2.643
3550	25.000	59.840	33.999	91.735	-60.058	-42.071	2.590
3550	25.000	59.840	33.999	91.735	-162.515	-42.071	2.590
3600	25.000	60.193	34.363	92.985	-162.420	-40.379	2.451
3700	25.000	60.878	35.071	95.485	-162.240	-36.995	2.185
3800	25.000	61.544	35.759	97.985	-162.074	-33.608	1.933
3900	25.000	62.194	36.428	100.485	-161.922	-30.237	1.694
3969.96	25.000	62.637	36.814	102.234	-161.821	-27.583	1.518
3969.96	25.000	62.637	36.814	102.234	-402.965	-27.583	1.518
4000	25.000	62.827	37.080	102.985	402.772	-25.026	1.367
4100	25.000	63.444	37.716	105.485	-402.14	-15.596	0.831
4200	25.000	64.046	[illegible]	107.985	[illegible]	-6.173	0.321
4300	25.000	64.635	[illegible]	110.485	-400.919	3.244	-0.165
4400	25.000	65.209	39.531	112.985	-400.327	12.632	-0.627
4500	25.000	65.771	40.108	115.485	-399.746	22.007	-1.069
4600	25.000	66.321	40.672	117.985	-399.175	31.369	-1.490
4700	25.000	66.858	41.223	120.485	-398.617	40.728	-1.894
4800	25.000	67.385	41.763	122.985	-398.070	50.073	-2.280
4900	25.000	67.900	42.291	125.485	-397.534	59.399	-2.649
5000	25.000	68.405	42.808	127.985	-397.006	68.725	-3.004
5100	25.000	68.900	43.315	130.485	-396.489	78.031	-3.344
5200	25.000	69.386	43.812	132.985	-395.983	87.330	-3.670
5300	25.000	69.862	44.299	135.485	-395.484	96.613	-3.984
5400	25.000	70.329	44.776	137.985	-394.996	105.896	-4.286
5500	25.000	70.788	45.245	140.485	-394.514	115.178	-4.577
5600	25.000	71.238	45.705	142.985	-394.042	124.429	-4.856
5700	25.000	71.681	46.157	145.485	-393.579	133.693	-5.126
5800	25.000	72.116	46.601	147.985	-393.121	142.930	-5.385
5900	25.000	72.543	47.037	150.485	-392.673	152.176	-5.637
6000	25.000	72.963	47.466	152.985	-392.231	161.408	-5.879

15 March 1963 HLS

TITANIUM DIBORIDE (TiB_2) (CONDENSED PHASE) gfw = 69.54

$\Delta H^o_{f298.15} = -66.85$ Kcal gfw^{-1}

$S^o_{298.15} = 6.7 \pm 0.5$ cal degK^{-1} gfw^{-1}

$T_m = 3193^oK$

$\Delta H_m = 22.032 \pm 50$ Kcal gfw^{-1}

$H^o_{298.15} - H^o_0 = 1.381$ Kcal gfw^{-1}

$298.15^oK \leq T \leq 3193^oK$

$C^o_p = 14.99 + 3.74 \times 10^{-3}T - 4.98 \times 10^5 T^{-2}$ cal degK^{-1} gfw^{-1}

$C^o_p = 25.0$ cal deg K^{-1} gfw^{-1} (estd.) above T = 3193°K

Structure

TiB_2 is of the hexagonal, AlB_2(C32) structure with a narrow homogeneity range.

Heat of Formation

Calorimetric value of Epel'baum and Starostina[1] were chosen. It was consistent within about ± 3 Kcal with vaporization data and nitride equilibria. See text for details.

Heat Capacity and Entropy

Low temperature data were estimated. High temperature data from Kelley,[2] in agreement with other data, were used. See volume 1, this report for details. Heat capacity above melting point was estimated.

Melting and Heat of Sublimation

Melting point by Post *et al.*[3] Heat of fusion estimated.

References

1. Epel'baum, V. A. and M. I. Starostina, Chem. Abst. 54, 23701 (1960).
2. Kelley, K. K., Bur. Mines, Bull. 584 (1960).
3. Post, B., F. W. Glaser and D. Moskowitz, Acta. Met. 2, 20-5 (1954).

TITANIUM DIBORIDE (TiB_2) (CONDENSED PHASE) GFW = 69.54

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw			Kcal gfw.			
	C^o_p	S^o_T	$-(F^o_T - H^o_{298})/T$	$H^o_T - H^o_{298}$	ΔH_f	ΔF_f	Log K_p
298.15	± 0.300	±0.500	±0.500	±0.000			
1000	± 0.650	±0.863	±0.652	±0.211			
2000	± 1.500	±1.556	±0.951	±1.211			
3000	± 2.000	±2.367	±1.297	±3.211			
3193	± 2.000	±2.492	±1.365	±3.597			
3193	± 3.000	±4.058	±1.365	±8.597			
4000	± 3.000	±4.734	±1.979	±11.018			
5000	± 3.000	±5.403	±2.600	±14.018			
6000	± 3.000	±5.950	±3.114	±17.018			

TABLE 95

ZIRCONIUM DIBORIDE CONDENSED PHASE B_2Zr

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Zr from 0° to 2125°K, Liquid Zr from 2125° to 4644°K, Gaseous Zr from 4644° to 6000°K, Solid B from 0° to 2450°K, Liquid B from 2450° to 3970°K, Gaseous B from 3970° to 6000°K, Solid ZrB_2 from 0° to 3313°K, Liquid ZrB_2 from 3313° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.590	-72.697	-72.697	INFINITE
298.15	11.530	8.590	8.590	0.000	-73.000	-71.961	52.746
300	11.596	8.662	8.590	0.021	-73.002	-71.957	52.418
400	14.077	12.379	9.080	1.320	-73.008	-71.606	39.122
500	15.467	15.681	10.077	2.802	-73.037	-71.251	31.142
600	16.427	18.590	11.259	4.399	-73.091	-70.892	25.821
700	17.185	21.181	12.494	6.081	-73.162	-70.518	22.016
800	17.835	23.519	13.729	7.832	-73.251	-70.135	19.159
900	18.422	25.654	14.937	9.646	-73.352	-69.739	16.934
1000	18.970	27.624	16.108	11.516	-73.462	-69.331	15.152
1100	19.493	29.457	17.240	13.439	-73.577	-68.913	13.691
1135	19.671	30.070	17.626	14.124	-73.618	-68.764	13.240
1135	19.671	30.070	17.626	14.124	-74.533	-68.764	13.240
1200	19.998	31.175	18.330	15.414	-74.595	-68.433	12.463
1300	20.491	32.795	19.381	17.438	-74.675	-67.917	11.417
1400	20.975	34.351	20.394	19.511	-74.736	-67.394	10.520
1500	21.452	35.795	21.373	21.633	-74.772	-66.866	9.742
1600	21.925	37.194	22.318	23.802	-74.783	-66.341	9.061
1700	22.393	38.537	23.233	26.018	74.765	-65.812	8.460
1800	22.859	39.831	24.119	28.280	-74.717	-65.287	7.927
1900	23.322	41.079	24.979	30.589	-74.638	-64.767	7.450
2000	23.784	42.287	25.815	32.945	-74.524	-64.248	7.020
2100	24.243	43.458	26.627	35.346	-74.375	-63.741	6.633
2125	24.358	43.746	26.827	35.954	-74.332	-63.616	6.542
2125	24.358	43.746	26.827	35.954	-79.232	-63.616	6.542
2200	24.702	44.597	27.418	37.793	-79.099	-63.065	6.265
2300	25.159	45.705	28.189	40.286	-78.888	-62.342	5.924
2400	25.615	46.785	28.942	42.825	-78.637	-61.626	5.612
2450	25.843	47.316	29.311	44.112	-78.496	-61.171	5.456
2450	25.843	47.316	29.311	44.112	-89.766	-61.171	5.456
2500	26.071	47.840	29.677	45.409	-89.619	-60.595	5.297
2600	26.526	48.872	30.395	48.039	-89.289	-59.438	4.996
2700	26.981	49.881	31.098	50.715	-88.913	-58.299	4.719
2800	27.435	50.871	31.787	53.435	-88.493	-57.172	4.462
2900	27.888	51.841	32.462	56.202	-88.026	-56.061	4.225
3000	28.347	52.795	33.123	59.013	-87.515	-54.964	4.004
3100	28.795	53.731	33.773	61.870	-86.958	-53.885	3.799
3200	29.247	54.653	34.411	64.772	-86.356	-52.830	3.608
3300	29.700	55.559	35.038	67.719	-85.709	-51.794	3.430
3313	29.758	55.676	35.119	68.106	-85.620	-51.658	3.408
3313	29.758	63.222	35.119	93.106	-60.620	-51.658	3.408
3400	29.758	63.994	35.848	95.695	-60.033	-51.434	3.306
3500	29.758	64.856	36.665	98.671	-59.357	-51.192	3.196
3600	29.758	65.695	37.460	101.646	-58.682	-50.964	3.094
3700	29.758	66.510	38.234	104.622	-58.006	-50.759	2.998
3800	29.758	67.304	38.988	107.598	-57.330	-50.569	2.908
3900	29.758	68.077	39.724	110.574	-56.654	-50.403	2.824
3969.96	29.758	68.606	40.229	112.656	-56.180	-50.292	2.768
3969.96	29.758	68.606	40.229	112.656	-297.324	-50.292	2.768
4000	29.758	68.830	40.443	113.550	-296.968	-48.420	2.645
4100	29.758	69.565	41.144	116.525	-295.791	-42.225	2.251
4200	29.758	70.262	41.829	119.501	-294.611	-36.053	1.876
4300	29.758	70.982	42.499	122.477	-293.433	-29.901	1.520
4400	29.758	71.666	43.154	125.453	-292.257	-23.790	1.182
4500	29.758	72.335	43.[illegible]	128.429	-291.081	-17.699	0.860
4600	29.758	72.989	44.423	131.404	-289.906	-11.645	0.553
4644.05	29.758	73.273	44.695	132.715	-289.389	-8.977	0.422
4644.05	29.758	73.273	44.695	132.715	-424.843	-8.977	0.422
4700	29.758	73.629	45.037	134.380	-424.240	-3.966	0.184
4800	29.758	74.255	45.640	137.356	-423.169	4.962	-0.226
4900	29.758	74.869	46.230	140.332	-422.106	13.867	-0.618
5000	29.758	75.470	46.809	143.308	-421.047	22.760	-0.995
5100	29.758	76.060	47.377	146.283	-419.996	31.616	-1.355
5200	29.758	76.637	47.934	149.259	-418.953	40.469	-1.701
5300	29.758	77.204	48.481	152.235	-417.914	49.282	-2.032
5400	29.758	77.760	49.018	155.211	-416.882	58.090	-2.351
5500	29.758	78.307	49.545	158.187	-415.853	66.887	-2.658
5600	29.758	78.843	50.064	161.162	-414.833	75.646	-2.952
5700	29.758	79.369	50.573	164.138	-413.819	84.405	-3.236
5800	29.758	79.887	51.074	167.114	-412.806	93.129	-3.509
5900	29.758	80.396	51.567	170.090	-411.802	101.846	-3.772
6000	29.758	80.896	52.052	173.066	-410.802	110.552	-4.027

15 March 1963 HLS

ZIRCONIUM DIBORIDE (ZrB_2) (CONDENSED PHASE) gfw = 112.86

$\Delta H^o_{f298.15}$ = -73.0 Kcal gfw^{-1}

$S^o_{298.15}$ = 8.59 cal degK^{-1} gfw^{-1}

T_m = 3313°K

ΔH_m = 25.000 ± 5.000 Kcal gfw^{-1}

$H^o_{298.15}-H^o_0$ = 1.590 Kcal gfw^{-1}

$C^o_p = 14.888 + 4.50 \times 10^{-3}T - 4.178 \times 10^5 T^{-2}$ cal degK^{-1} gfw^{-1}

$298.15°K \leq T \leq 3313°K$

Structure

ZrB_2 is of the hexagonal AlB_2 (C32) structure with a narrow homogeneity range.

Heat of Formation

The value chosen is based primarily on three calorimetric determinations[1, 2, 3] and is in general agreement with vaporization studies.[4, 5]

Heat Capacity and Entropy

Low temperature data by Westrum and Feick.[6] This data was joined by the Shomate method to Margrave[7] and Southern Research Institute data.[8]

Melting and Heat of Sublimation

Melting temperature from Glaser and Post.[9] Heat of fusion estimated.

References

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ZIRCONIUM DIBORIDE (ZrB_2) (CONDENSED PHASE) GFW = 112.86

SUMMARY OF UNCERTAINTY ESTIMATES

T,°K	C^o_p (cal/°K gfw)	S^o_T (cal/°K gfw)	$-(F^o_T - H^o_{298})/T$ (cal/°K gfw)	$H^o_T - H^o_{298}$ (kcal/gfw)	ΔH^o_f (kcal/gfw)	ΔF^o_f (kcal/gfw)	Log K_p
298.15	± 0.300	± 0.050	± 0.050	± 0.000	± 2.000		
1000	± 1.000	± 0.898	± 0.338	± 0.561			
2000	± 2.000	± 1.879	± 0.849	± 2.061			
3000	± 2.000	± 2.690	± 1.336	± 4.061			
3313	± 2.000	± 2.888	± 1.474	± 4.687			
3313	± 4.000	± 4.398	± 1.474	± 9.687			
4000	± 4.000	± 5.151	± 2.043	±12.435			
5000	± 4.000	± 6.044	± 2.757	±16.435			
6000	± 4.000	± 6.773	± 3.368	±20.435			

TABLE 96

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p

Solid Be from 0° to 1556°K, Liquid Be from 1556° to 2768°K, Gaseous Be from 2768° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-0.467			
298.15	3.932	2.282	2.282	0.000			
300	3.951	2.307	2.283	0.007			
400	4.773	3.365	2.447	0.447			
500	5.260	4.687	2.787	0.950			
600	5.588	5.676	3.186	1.494			
700	5.846	6.557	3.606	2.066			
800	6.072	7.353	4.025	2.662			
900	6.287	8.081	4.437	3.280			
1000	6.508	8.754	4.835	3.919			
1100	6.720	9.384	5.219	4.582			
1200	6.938	9.978	5.590	5.266			
1300	7.156	10.542	5.949	5.971			
1400	7.374	11.080	6.296	6.697			
1500	7.592	11.596	6.633	7.445			
1556	7.714	11.877	6.817	7.874			
1556	6.878	14.139	6.817	11.394			
1600	6.901	14.331	7.021	11.697			
1700	6.952	14.751	7.464	12.390			
1800	7.004	15.150	7.880	13.088			
1900	7.055	15.530	8.273	13.791			
2000	7.107	15.893	8.645	14.499			
2100	7.158	16.241	9.000	15.212			
2200	7.209	16.575	9.337	15.930			
2300	7.261	16.897	9.659	16.654			
2400	7.312	17.207	9.968	17.387			
2500	7.364	17.507	10.264	18.116			
2600	7.415	17.796	10.548	18.855			
2700	7.466	18.077	10.822	19.599			
2767.61	7.501	18.281	11.002	20.108			
2767.61	4.994	43.[illegible]17	11.002	90.277			
2800	4.997	43.475	11.376	90.437			
2900	5.007	43.851	12.493	90.937			
3000	5.021	44.021	13.542	91.438			
3100	5.037	44.186	14.528	91.941			
3200	5.057	44.346	15.457	92.446			
3300	5.081	44.502	16.334	92.943			
3400	5.109	44.654	17.165	93.452			
3500	5.142	44.803	17.953	93.975			
3600	5.179	44.948	18.700	94.491			
3700	5.221	45.090	19.412	95.010			
3800	5.268	45.230	20.089	95.535			
3900	5.320	45.368	20.736	96.064			
4000	5.378	45.503	21.353	96.599			
4100	5.440	45.637	21.944	97.140			
4200	5.508	45.769	22.510	97.687			
4300	5.581	45.899	23.052	98.242			
4400	5.658	46.028	23.573	98.804			
4500	5.741	46.156	24.073	99.373			
4600	5.828	46.283	24.554	99.952			
4700	5.919	46.410	25.019	100.539			
4800	6.014	46.535	25.465	101.136			
4900	6.113	46.660	25.896	101.742			
5000	6.215	46.785	26.313	102.358			
5100	6.320	46.909	26.[illegible]16	102.985			
5200	6.428	47.033	27.[illegible]	103.622			
5300	6.538	47.156	27.482	104.271			
5400	6.649	47.279	27.848	104.930			
5500	6.763	47.402	28.202	105.601			
5600	6.877	47.525	28.546	106.283			
5700	6.993	47.648	28.880	106.976			
5800	7.108	47.771	29.205	107.681			
5900	7.224	47.893	29.520	108.398			
6000	7.340	48.016	29.828	109.126			

15 September 1962 RCF

BERYLLIUM (Be) (REFERENCE STATE) gfw = 9.013

0 °K to 1556 °K Crystal

1556 °K to 2767.61 °K Liquid

2767.61 °K to 6000 °K Ideal Monatomic Gas

$\Delta H^\circ_{f0} = 0$ Kcal gfw^{-1}

$\Delta H^\circ_{f298.15} = 0$ kcal gfw^{-1}

$\Delta H^\circ_{s298.15} = 78.0$ kcal gfw^{-1}

$S^\circ_{298.15} = 2.282 \pm .020$ cal degK^{-1}gfw^{-1}

$T_m = 1556° \pm 3$ °K

$\Delta H_m = 3.520 \pm .080$ Kcal gfw^{-1}

$T_b = 2768° \pm 35$ °K

$\Delta H_v = 70.169 \pm .870$ Kcal gfw^{-1}

$H^\circ_{298.15} - H^\circ_0 = .467$ Kcal gfw^{-1}

$C^\circ_p = 4.322 + 2.18 \times 10^{-3}$ T cal deg K^{-1} gfw^{-1} 600 °K $\leq$ T $\leq$ 1560 °K

$C^\circ_p = 6.079 + 5.138 \times 10^{-4}$ T cal deg K^{-1} gfw^{-1} 1560 °K $\leq$ T $\leq$ 2200 °K

(latter equation extrapolated to 2768°K).

Structure

H. C. P. to about 20°K below T_m, B. C. C. to T_m

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Heat capacities from Kantor, et al[1].

Melting

Based on several determinations[2].

Vaporization

Based on earlier report[2].

References

1. Kantor, P., et al, Fiz. Met. i. Metalloved 10, 835 (1960).

2. Barriault, R. J., et al, Thermodynamics of Certain Refractory Compounds, ASD TR 61-260 Pt. I (May 1962).

BERYLLIUM (Be) (REFERENCE STATE) GFW = 9.013

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal °K gfw)	S_T (cal °K gfw)	$-(F_T - H_{298})/T$ (cal °K gfw)	$H_T - H_{298}$ (Kcal gfw)	ΔH_f (Kcal gfw)	ΔF_f (Kcal gfw)	Log K_p
298.15	± 0.050	± 0.020	± 0.020	± 0.000			
1000	± 0.050	± 0.070	± 0.030	± 0.040			
1556	± 0.050	± 0.100	± 0.060	± 0.060			
1556	± 0.100	± 0.155	± 0.060	± 0.140			
2000	± 0.150	± 0.185	± 0.080	± 0.200			
2767.61	± 0.300	± 0.255	± 0.120	± 0.320			
2767.61	± 0.001	± 0.002	± 0.003	± 0.001			
3000	± 0.001	± 0.002	± 0.00[illegible]	± 0.001			
4000	± 0.002	± 0.003	± 0.003	± 0.002			
5000	± 0.002	± 0.003	± 0.003	± 0.004			
6000	± 0.002	± 0.003	± 0.004	± 0.005			

TABLE 97

BERYLLIUM IDEAL MONATOMIC GAS **Be**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p
Solid Be from 0° to 1556°K, Liquid Be from 1556° to 2768°K, Gaseous Be from 2768° to 6000°K

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.481	76.986	76.986	INFINITE
298.15	4.968	32.545	32.545	0.000	78.000	68.977	-50.559
300	4.968	32.576	32.545	0.009	78.002	68.921	-50.206
400	4.968	34.005	32.740	0.506	78.059	65.883	-35.995
500	4.968	35.114	33.108	1.003	78.053	62.839	-27.466
600	4.968	36.020	33.520	1.500	78.006	59.800	-21.781
700	4.968	36.785	33.933	1.996	77.930	56.700	-17.724
800	4.968	37.449	34.332	2.493	77.831	53.754	-14.684
900	4.968	38.034	34.712	2.990	77.710	50.752	-12.324
1000	4.968	38.557	35.070	3.487	77.568	47.765	-10.439
1100	4.968	39.031	35.409	3.984	77.402	44.791	-8.899
1200	4.968	39.463	35.729	4.481	77.215	41.833	-7.618
1300	4.968	39.861	36.032	4.977	77.006	38.892	-6.538
1400	4.968	40.229	36.319	5.474	76.777	35.968	-5.615
1500	4.968	40.572	36.591	5.971	76.526	33.063	-4.817
1556	4.968	40.754	36.738	6.249	76.375	31.443	-4.416
1556	4.968	40.754	36.738	6.249	72.855	31.443	-4.416
1600	4.968	40.892	35.850	6.468	72.771	30.274	-4.135
1700	4.968	41.194	37.097	6.965	72.575	27.624	-3.551
1800	4.968	41.478	37.322	7.461	72.373	24.986	-3.034
1900	4.968	41.746	37.558	7.958	72.165	22.359	-2.572
2000	4.969	42.001	37.774	8.455	71.956	19.742	-2.157
2100	4.969	42.244	37.981	8.952	71.740	17.140	-1.784
2200	4.970	42.475	38.180	9.449	71.519	14.545	-1.445
2300	4.972	42.696	38.371	9.946	71.292	11.962	-1.137
2400	4.974	42.907	38.556	10.443	71.061	9.389	-0.855
2500	4.977	43.110	38.734	10.941	70.875	6.825	-0.597
2600	4.982	43.306	38.906	11.439	70.584	4.269	-0.359
2700	4.988	43.494	39.073	11.937	70.338	1.722	-0.139
2767.61	4.994	43.617	39.182	12.277	70.169	0.000	0.000
2767.61	4.994	43.617	39.182	12.277			
2800	4.997	43.675	39.234	12.437			
2900	5.007	43.851	39.390	12.937			
3000	5.021	44.021	39.542	13.438			
3100	5.037	44.186	39.689	13.941			
3200	5.057	44.346	39.832	14.446			
3300	5.081	44.502	39.971	14.953			
3400	5.109	44.654	40.106	15.462			
3500	5.142	44.803	40.238	15.975			
3600	5.179	44.948	40.367	16.491			
3700	5.221	45.090	40.493	17.010			
3800	5.268	45.230	40.616	17.535			
3900	5.320	45.368	40.736	18.064			
4000	5.378	45.503	40.853	18.599			
4100	5.440	45.637	40.968	19.140			
4200	5.508	45.769	41.081	19.687			
4300	5.581	45.899	41.192	20.242			
4400	5.658	46.028	41.300	20.804			
4500	5.741	46.156	41.407	21.373			
4600	5.828	46.283	41.511	21.952			
4700	5.919	46.410	41.614	22.539			
4800	6.014	46.535	41.715	23.136			
4900	6.113	46.660	41.815	23.742			
5000	6.215	46.785	41.913	24.358			
5100	6.320	46.909	42.01[illegible]	24.985			
5200	6.428	47.033	42.105	25.622			
5300	6.538	47.156	42.199	26.271			
5400	6.649	47.279	42.292	26.930			
5500	6.763	47.402	42.384	27.601			
5600	6.877	47.525	42.475	28.283			
5700	6.993	47.648	42.565	28.976			
5800	7.108	47.771	42.653	29.681			
5900	7.224	47.893	42.741	30.398			
6000	7.340	48.016	42.828	31.126			

RCF

BERYLLIUM, MONATOMIC (Be) (IDEAL GAS) gfw = 9.013

ΔH^o_{f0} = 76.986 kcal fgw^{-1}

$\Delta H^o_{f298.15}$ = 78.000 $\pm$ .500 kcal gfw^{-1}

Ground State Configuration = $^1S_0$

$S^o_{298.15}$ = 32.545 $\pm$ .002 cal deg K^{-1}gfw^{-1}

$H^o_{298.15} - H^o_0$ = 1.481 Kcal gfw-1

Electronic levels and multiplicities

All levels from Moore[1]

Heat of Formation

Based on previous report.[2]

Heat Capacity and Entropy

Calculated using monatomic-gas program.

References

1. Moore, C., NBS Circular 467, Vol. 1 (15 June 1949).

2. Barriault, R. J. et al, Thermodynamics of Certain Refractory Compounds, ASD TR 61-760, Part I (May 1962)

BERYLLIUM, MONATOMIC (Be) (IDEAL GAS) GFW = 9.013

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S_T (cal/°K gfw)	$-(F_T - H_{298})/T$ (cal/°K gfw)	$H_T - H_{298}$ (kcal gfw)	ΔH_f (kcal gfw)	ΔF_f (kcal gfw)	Log K_p
298.15	±0.000	±0.002	±0.002	±0.000	±0.500	±0.510	±0.370
1000	±0.000	±0.002	±0.002	±0.000	±0.540	±0.530	±0.120
1556	±0.000	±0.002	±0.002	±0.000	±0.560	±0.580	±0.080
1556	±0.000	±0.055	±0.002	±0.080	±0.640	±0.580	±0.108
2000	±0.000	±0.057	±0.003	±0.080	±0.700	±0.670	±0.070
2767.61	±0.000	±0.057	±0.003	±0.080	±0.870	±0.840	±0.070
2767.61	±0.000	±0.386	±0.003	±0.950			
3000	±0.001	±0.388	±0.003	±0.951			
4000	±0.002	±0.391	±0.003	±0.952			
5000	±0.002	±0.391	±0.003	±0.954			
6000	±0.002	±0.391	±0.004	±0.955			

BERYLLIUM OXIDE

CONDENSED PHASE

BeO

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Be from 0° to 1556°K, Liquid Be from 1556° to 2768°K, Gaseous Be from 2768° to 6000°K, Gaseous O_2. Solid BeO from 0° to 2820°K, Liquid BeO from 2820° to 4500°K.

T, °K	cal/°K gfw C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	Kcal/gfw $H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-0.687	-142.283	-142.283	INFINITE
298.15	6.105	3.376	3.376	0.000	-143.100	-136.120	99.774
300	6.148	3.414	3.376	0.011	-143.103	-136.077	99.127
400	8.803	5.467	3.643	0.730	-143.178	-133.722	73.059
500	9.310	7.412	4.204	1.604	-143.173	-131.355	57.412
600	10.128	9.186	4.889	2.578	-143.121	-128.997	46.985
700	10.714	10.793	5.619	3.622	-143.038	-126.649	39.540
800	11.154	12.254	6.359	4.716	-142.939	-124.314	33.959
900	11.498	13.588	7.089	5.849	-142.831	-121.991	29.622
1000	11.776	14.815	7.801	7.014	-142.718	-119.683	26.155
1100	12.005	15.948	8.491	8.203	-142.612	-117.386	23.321
1200	12.197	17.001	9.157	9.413	-142.510	-115.099	20.961
1300	12.361	17.984	9.798	10.641	-142.415	-112.818	18.965
1400	12.503	18.905	10.416	11.885	-142.329	-110.546	17.256
1500	12.628	19.772	11.011	13.142	-142.256	-108.276	15.775
1556	12.723	20.235	11.333	13.851	-142.221	-107.007	15.029
1556	12.723	20.235	11.333	13.851	-145.741	-107.007	15.029
1600	12.815	20.592	11.584	14.412	-145.676	-105.913	14.466
1700	13.024	21.375	12.137	15.704	-145.519	-103.432	13.297
1800	13.233	22.125	12.671	17.017	-145.348	-100.960	12.258
1900	13.442	22.846	13.188	18.351	-145.164	-98.499	11.330
2000	13.651	23.541	13.688	19.706	-144.967	-96.048	10.495
2100	13.860	24.212	14.174	21.081	-144.758	-93.605	9.741
2200	14.069	24.862	14.645	22.478	-144.534	-91.176	9.057
2300	14.278	25.492	15.103	23.895	-144.300	-88.753	8.433
2400	14.487	26.104	15.549	25.333	-144.051	-86.342	7.862
2500	14.696	26.699	15.982	26.792	-143.789	-83.940	7.338
2600	14.905	27.280	16.406	28.272	-143.515	-81.555	6.855
2700	15.114	27.846	16.819	29.774	-143.225	-79.175	6.408
2767.61	15.256	28.223	17.094	30.806	-143.023	-77.565	6.124
2767.61	15.256	28.223	17.094	30.806	-213.192	-77.565	6.124
2800	15.323	28.400	17.223	31.295	-213.014	-75.998	5.932
2820	15.365	28.509	17.303	31.602	-212.902	-75.039	5.815
2820	17.000	33.984	17.303	47.042	-197.462	-75.039	5.815
2900	17.000	34.459	17.769	48.402	-196.880	-71.551	5.392
3000	17.000	35.036	18.335	50.102	-196.158	-67.239	4.898
3100	17.000	35.593	18.8[illegible]	51.802	-19[illegible].439	-62.956	4.438
3200	17.000	36.133	19.414	53.502	-1[illegible] 725	-58.694	4.008
3300	17.000	36.656	19.928	55.202	-19[illegible].015	-54.455	3.606
3400	17.000	37.164	20.428	56.902	-193.308	-50.236	3.229
3500	17.000	37.656	20.913	50.602	-192.608	-46.038	2.875
3600	17.000	38.135	21.384	60.302	-191.913	-41.861	2.541
3700	17.000	38.601	21.844	62.002	-191.223	-37.702	2.227
3800	17.000	39.054	22.290	63.702	-190.541	-33.561	1.930
3900	17.000	39.496	22.726	65.402	-189.864	-29.433	1.650
4000	17.000	39.926	23.150	67.102	-189.195	-25.332	1.384
4100	17.000	40.[illegible]46	23.565	68.802	-1[illegible].534	-21.244	1.132
4200	17.000	40.7[illegible]6	23.970	70.502	-187.881	-17.171	0.893
4300	17.000	41.156	24.365	72.202	-187.238	-13.115	0.667
4400	17.000	41.547	24.751	73.902	-186.603	-9.072	0.451
4500	17.000	41.929	25.129	75.60[illegible]	-185.978	-5.049	0.245

RCF

BERYLLIUM OXIDE (BeO) (CONDENSED PHASE) gfw = 25.013

$\Delta H^\circ_{f298.15}$ = -143.100 ±Kcal gfw^{-1} $S^\circ_{298.15}$ = 3.376 ± .050 cal deg K^{-1}gfw^{-1}

T_m = 2820 °K ΔH_m = 15.440 ± .500 Kcal gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 0.687 Kcal gfw^{-1}

C°_p = 17 cal deg K^{-1}gfw^{-1} 2820°K ≤ T ≤ 4500 °K

Structure

Solid has hexagonal (wurtzite-type) structure.

Heat of Formation

Cosgrove and Snyder[1]

Heat Capacity and Entropy

Heat capacities of solid from Victor and Douglas[2] for T< 1500°K and from Kandyba, et al[3] for T> 1500°K.

Melting and Vaporization

Based on the mass spectrometric results of Chupka, et al[4].

References

1. Cosgrove, L.A. and P.E. Snyder, J. Am. Chem. Soc. 75, 3102 (1953).

2. Victor and Douglas, NBS Report 6484 (1959).

3. Kandyba, V. V., et al., Doklady Akad. Nauk SSSR 131, 566 (1960).

4. Chupka W.A., J. Berkowitz, and C.F. Giese, J. Chem. Phys. 30, 827 (1959).

BERYLLIUM MONOXIDE (BeO) (CONDENSED PHASE) GFW = 25.013

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal/gfw)	ΔH_f (Kcal/gfw)	ΔF_f (Kcal/gfw)	Log K_p
298.15	± 0.100	± 0.050	± 0.050	± 0.000	± 4.000	± 4.000	± 2.950
1000	± 0.300	± 0.150	± 0.080	± 0.070	± 4.110	± 4.110	± 0.900
2000	± 0.700	± 0.290	± 0.150	± 0.270	± 4.470	± 4.460	± 0.490
2820	± 1.580	± 0.444	± 0.220	± 0.630	± 5.500	± 5.460	± 0.420
2820	± 1.000	± 0.620	± 0.220	± 1.130	± 6.000	± 5.960	± 0.420
4000	± 2.000	± 1.140	± 0.420	± 2.900	± 7.780	± 6.530	± 0.360

BERYLLIUM OXIDE — IDEAL MOLECULAR GAS — BeO

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Be from 0° to 1556°K, Liquid Be from 1556° to 2768°K, Gaseous Be from 2768° to 6000°K; Gaseous O_2, Gaseous BeO.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.077	29.547	29.547	INFINITE
298.15	7.046	47.209	47.209	0.000	30.120	24.031	-17.614
300	7.049	47.252	47.209	0.013	30.119	23.993	-17.478
400	7.254	[illegible]	47.488	0.727	30.039	21.960	-11.998
500	7.510	50.952	48.021	1.465	29.908	19.956	-8.723
600	7.757	52.344	48.628	2.229	29.750	17.980	-6.549
700	7.970	53.556	49.248	3.016	29.576	16.031	-5.005
800	8.146	54.632	49.855	3.822	29.387	14.108	-3.854
900	8.289	55.600	50.440	4.644	29.184	12.213	-2.965
1000	8.406	56.480	51.001	5.479	29.967	10.337	-2.259
1100	8.504	57.285	51.536	6.324	28.729	8.484	-1.685
1200	8.588	58.029	52.046	7.179	28.476	6.654	-1.212
1300	8.665	58.720	52.534	8.042	28.206	4.845	-0.814
1400	8.737	59.364	52.999	8.912	27.918	3.058	-0.477
1500	8.810	59.970	53.443	9.789	27.611	1.296	-0.189
1556	8.852	60.290	53.681	10.284	27.446	0.320	-0.045
1556	8.852	60.290	53.681	10.284	23.912	0.320	-0.045
1600	8.885	60.541	53.869	10.674	23.806	-0.349	0.048
1700	8.966	61.082	54.278	11.567	23.564	-1.852	0.238
1800	9.052	61.597	54.670	12.467	23.322	-3.338	0.405
1900	9.146	62.088	54.048	13.377	23.082	-4.813	0.554
2000	9.246	62.560	55.412	14.297	22.844	-6.276	0.686
2100	9.353	63.014	55.763	15.227	22.608	-7.722	0.804
2200	9.465	63.451	56.103	16.167	22.375	-9.163	0.910
2300	9.582	63.875	56.431	17.120	22.145	-10.588	1.006
2400	9.703	64.285	56.750	18.084	21.920	-12.005	1.093
2500	9.827	64.684	57.060	19.061	21.700	-13.415	1.173
2600	9.951	65.072	57.360	20.049	21.482	-14.816	1.245
2700	10.076	65.450	57.653	21.051	21.272	-16.207	1.312
2767.61	10.159	65.700	57.847	21.737	21.128	-17.149	1.354
2767.61	10.159	65.700	57.847	21.737	-49.041	-17.149	1.354
2800	10.199	65.818	57.938	22.065	-49.025	-16.780	1.310
2900	10.320	66.179	58.216	23.091	-48.971	-15.627	1.178
3000	10.437	66.530	58.488	24.128	-48.912	-14.478	1.055
3100	10.551	66.875	58.753	25.178	-48.843	-13.333	0.940
3200	10.659	67.212	59.012	26.239	[illegible]	-12.187	0.832
3300	10.763	67.541	59.266	27.310	[illegible]	-11.051	0.732
3400	10.861	[illegible]	59.514	28.391	[illegible]	-9.908	0.637
3500	10.953	[illegible]	59.757	29.482	[illegible]	-8.772	0.548
3600	11.038	68.491	59.996	30.582	-48.413	-7.644	0.464
3700	11.118	68.794	60.229	31.690	-48.315	-6.506	0.384
3800	11.191	69.092	60.459	32.806	-48.217	-5.383	0.310
3900	11.258	69.384	60.684	33.929	-48.117	-4.255	0.238
4000	11.319	69.670	60.906	35.058	-48.019	-3.136	0.171
4100	11.374	69.950	61.123	36.193	-47.923	-2.012	0.107
4200	11.423	70.226	61.337	37.333	-47.830	-0.893	0.046
4300	11.467	70.495	61.547	38.478	-47.742	0.222	-0.011
4400	11.506	70.760	61.754	39.628	-47.657	1.335	-0.066
4500	11.540	71.019	61.957	40.780	-47.580	2.445	-0.119
4600	11.570	71.274	62.157	41.937	-47.510	3.555	-0.169
4700	11.595	71.523	62.354	43.096	-47.449	4.670	-0.217
4800	11.617	71.768	62.548	44.257	-47.398	5.770	-0.263
4900	11.635	72.008	62.73	45.421	-47.357	6.874	-0.307
5000	11.649	72.244	62.927	46.586	-47.328	7.985	-0.349
5100	11.661	72.476	63.113	47.752	-47.314	9.088	-0.389
5200	11.669	72.703	63.295	48.920	-47.313	10.199	-0.429
5300	11.676	72.926	63.475	50.088	-47.331	11.300	-0.466
5400	11.680	73.145	63.653	51.257	-47.364	12.403	-0.502
5500	11.682	73.360	63.828	52.427	-47.418	13.505	-0.537
5600	11.682	73.572	64.001	53.597	-47.493	14.614	-0.570
5700	[illegible]	73.779	64.171	54.766	-47.594	15.722	-0.603
5800	[illegible]	73.983	64.339	55.936	-47.720	16.838	-0.634
5900	11.674	74.184	64.505	57.105	-47.879	17.942	-0.665
6000	11.670	74.381	64.669	58.274	-48.071	19.062	-0.694

RCF

BERYLLIUM OXIDE (BeO) (IDEAL MOLECULAR GAS) gfw = 25.013

ΔH°_{f0} = 29.547 Kcal gfw^{-1} $\Delta H^\circ_{f298.15}$ = 30.120 ± 3.000 Kcal gfw^{-1}

Ground State Configuration = $^1\Sigma^+$ $S^\circ_{298.15}$ = 47.209 cal deg K^{-1}gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 2.077 Kcal gfw^{-1}

Heat of Formation

Derived from data of Chupka et al[1].

Heat Capacity and Entropy

Calculated using diatomic gas program. Spectroscopic constants were from Herzberg.[2] Stretching constants, D_e values, not given by Herzberg were estimated with Dunham[3] equations.

References

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2. Herzberg, G., Spectra of Diatomic Molecules, Van Nostrand, N.Y. (1950).
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TABLE 100

BERYLLIUM CARBIDE CONDENSED PHASE Be_2C

Reference State for calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Be from 0° to 1556°K, Liquid Be from 1556° to 2767°K, Gaseous Be from 2767° to 6000°K; Solid C; Solid Be_2C from 0° to 2400°K, Liquid Be_2C from 2400° to 3500°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0							
298.15	10.340	4.000	4.000	0.000	-23.800	-23.227	17.025
300	10.350	4.064	4.000	0.019	-23.799	-23.222	16.917
400	10.860	7.111	4.412	1.080	-23.864	-23.027	12.581
500	11.371	9.590	5.207	2.191	-24.078	-22.793	9.963
600	11.882	11.708	6.118	3.354	-24.381	-22.512	8.200
700	12.392	13.578	7.053	4.568	-24.736	-22.172	6.922
800	12.903	15.266	7.976	5.832	-25.123	-21.782	5.950
900	13.413	16.815	8.873	7.148	-25.530	-21.337	5.181
1000	13.924	18.255	9.740	8.515	-25.947	-20.850	4.557
1100	14.435	19.606	10.576	9.933	-26.378	-20.322	4.037
1200	14.945	20.884	11.382	11.402	-26.813	-19.755	3.598
1300	15.456	22.100	12.160	12.922	-27.252	-19.150	3.219
1400	15.966	23.264	12.912	14.493	-27.689	-18.511	2.890
1500	16.477	24.383	13.640	16.115	-28.127	-17.839	2.599
1556	16.763	24.992	14.037	17.046	-28.372	-17.448	2.451
1556	16.763	24.992	14.037	17.046	-35.412	-17.448	2.451
1600	16.988	25.463	14.345	17.788	-35.528	-16.939	2.314
1700	17.498	26.508	15.030	19.513	-35.763	-15.768	2.027
1800	18.009	27.523	15.696	21.288	-35.963	-14.586	1.771
1900	18.519	28.510	16.345	23.114	-36.125	-13.394	1.541
2000	19.030	29.473	16.977	24.992	-36.248	-12.194	1.332
2100	19.541	30.414	17.595	26.920	-36.333	-10.984	1.143
2200	20.051	31.335	18.198	28.900	-36.380	-9.773	0.971
2300	20.562	32.237	18.789	30.931	-36.389	-8.565	0.814
2400	21.072	33.123	19.368	33.012	-36.369	-7.350	0.669
2400	21.072	40.623	19.368	51.012	-18.369	-7.350	0.669
2500	21.072	41.483	20.235	53.120	-18.315	-6.890	0.602
2600	21.072	42.310	21.069	55.227	-18.285	-6.437	0.541
2700	21.072	43.105	21.870	57.334	-18.266	-5.980	0.484
2767.61	21.072	43.626	22.395	58.759	-18.265	-5.669	0.448
2767.61	21.072	43.626	22.395	58.759	-158.603	-5.669	0.448
2800	21.072	43.871	22.642	59.441	-158.436	-3.900	0.304
2900	21.072	44.611	23.387	61.548	-157.933	1.610	-0.121
3000	21.072	45.325	24.107	63.656	-157.432	7.106	-0.518
3100	21.072	46.016	24.802	65.763	-156.937	12.585	-0.887
3200	21.072	46.685	25.476	67.870	-156.448	18.043	-1.232
3300	21.072	47.334	26.128	69.977	-155.945	23.482	-1.555
3400	21.072	47.963	26.761	72.084	-155.467	28.917	-1.859
3500	21.072	48.573	27.376	74.192	-155.018	34.335	-2.144

$\Delta H^\circ_{f298.15} = -23.8 \pm 1.8$ kcal gfw^{-1}

$S^\circ_{298.15} = 4.0 \pm 1.0$ cal deg K^{-1} gfw^{-1}

T_m = 2400°K

ΔH_m = 18.0 kcal gfw^{-1}

$C^\circ_p = 8.818 + 5.106 \times 10^{-3} T$ cal deg K^{-1} gfw^{-1} $\quad 298.15°K \le T \le 2400°K$

$C^\circ_p = 21.072$ cal deg K^{-1} gfw^{-1} $\quad 2400°K \le T \le 3500°K$

Structure

Face-centered-cubic C1-type: a = 4.33 kX.

Heat of Formation

Third Law calculation of Pollock's[1] data yields -23.8 ± 1.8 kcal gfw^{-1}.

Heat Capacity and Entropy

The heat-capacity equation of Neely *et al*[2] has been extrapolated to 2400°K. A constant heat capacity of 21.072 cal degK^{-1} gfw^{-1} has been used to 3500°K. An entropy value of 4.0 ± 1 is based on Krikorian's[3] estimate of ΔF_{298} and ΔH_{298}.

Melting and Vaporization

The melting point of 2400 ± 30°K is based upon the Brewer *et al*[4] value of 2373°K and Gaev's[5] reported decomposition at 2423°K.

References

1. Pollock, B., J. Phys. Chem. 63, 587 (1959).
2. Neely, J., C. Teeter, and J. Trice, J. Am. Ceram. Soc. 33, 363 (1950).
3. Krikorian, O., UCRL 2888 (1955).
4. Brewer, L., L. Bromley, P. Gilles, and N. Lofgren, The Chemistry and Metallurgy of Miscellaneous Materials, In: Thermodynamics, McGraw-Hill, New York (1950).
5. Gaev, I., AEC-TR-3036, Transl. from Zh. Neorg. Khim. 1, 196 (1956).

BERYLLIUM CARBIDE (Be_2C) (CONDENSED PHASE) GFW = 30.037

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal/gfw)	ΔH°_f (Kcal/gfw)	ΔF°_f (Kcal/gfw)	Log K_p
298.15	± 0.775	± 1.000	± 1.000	± 0.000	± 1.800		
500	± 0.852	± 1.419	± 1.091	± 0.164			
1000	± 1.044	± 2.069	± 1.430	± 0.638			
1500	± 1.235	± 2.528	± 1.723	± 1.208			
2000	± 1.427	± 2.910	± 1.973	± 1.874			
2400	± 1.580	± 3.184	± 2.152	± 2.475			
2400	± 3.000	± 4.684	± 2.152	± 6.075			
2500	± 3.000	± 4.806	± 2.256	± 6.375			
3000	± 3.000	± 5.353	± 2.728	± 7.875			
3500	± 3.000	± 5.815	± 3.137	± 9.375			

TABLE 101

DIMERIC BERYLLIUM OXIDE   IDEAL MOLECULAR GAS Be_2O_2

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Be from 0° to 1556°K, Liquid Be from 1556° to 2768°K, Gaseous Be from 2768° to 6000°K, Gaseous O_2, Gaseous Be_2O_2

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-3.000	-101.691	-101.691	INFINITE
298.15	10.831	58.562	58.562	0.000	-101.700	-103.188	75.635
300	10.866	58.629	58.562	0.020	-101.707	-103.197	75.175
400	12.712	62.012	59.011	1.200	-102.117	-103.633	56.620
500	14.265	65.022	59.918	2.552	-102.502	-103.965	45.441
600	15.461	67.734	60.998	4.041	-102.857	-104.225	37.962
700	16.356	70.188	62.139	5.634	-103.185	-104.428	32.602
800	17.026	72.418	63.286	7.305	-103.504	-104.584	28.570
900	17.533	74.454	64.416	9.034	-103.825	-104.698	25.423
1000	17.922	76.323	65.514	10.808	-104.157	-104.777	22.898
1100	18.225	78.046	66.576	12.616	-104.514	-104.825	20.826
1200	18.464	79.642	67.599	14.451	-104.895	-104.839	19.093
1300	18.657	81.128	68.584	16.307	-105.306	-104.821	17.621
1400	18.813	82.516	69.530	18.181	-105.748	-104.769	16.354
1500	18.942	83.819	70.439	20.069	-106.226	-104.679	15.251
1556	19.003	84.513	70.932	21.132	-106.512	-104.613	14.693
1556	19.003	84.513	70.932	21.132	-113.580	-104.613	14.693
1600	19.048	85.045	71.314	21.969	-113.735	-104.361	14.254
1700	19.138	86.203	72.156	23.878	-11[illegible].095	-103.764	13.339
1800	19.214	87.299	72.967	25.796	-114.462	-103.147	12.523
1900	19.279	88.339	73.749	27.721	-114.837	-102.509	11.791
2000	19.335	89.330	74.504	29.652	-115.222	-101.852	11.129
2100	19.383	90.274	75.232	31.588	-115.618	-101.169	10.528
2200	19.426	91.177	75.937	33.528	-116.025	-100.472	9.981
2300	19.463	92.041	76.618	35.473	-116.444	-99.757	9.479
2400	19.495	92.870	77.278	37.421	-116.874	-99.019	9.016
2500	19.524	93.667	77.918	39.372	-117.319	-98.268	8.590
2600	19.550	94.433	78.539	41.325	-117.776	-97.498	8.195
2700	19.573	95.1[illegible]1	79.141	43.282	-118.245	-96.710	7.828
2767.61	1[illegible].587	95.6[illegible]7	79.540	44.613	-118.572	-96.164	7.592
2767.61	19.587	95.657	79.540	44.613	-258.882	-96.164	7.592
2800	19.594	95.884	79.726	45.240	-258.877	-94.280	7.359
2900	19.612	96.572	80.295	47.200	-258.865	-88.401	6.662
3000	19.629	97.237	80.849	49.163	-258.856	-82.518	6.011
3100	19.644	97.881	81.388	51.126	-258.856	-76.637	5.403
3200	19.658	98.505	81.913	63.091	-258.863	-70.762	4.833
3300	19.671	99.110	82.425	55.058	-258.875	-64.889	4.297
3400	19.682	99.697	82.925	57.026	-[illegible].495	-59.010	3.793
3500	19.693	100.268	83.412	58.994	-25[illegible]	-53.123	3.317
3600	19.702	100.823	83.888	60.964	-258.967	-47.250	2.868
3700	19.711	101.363	84.353	62.935	-259.015	-41.364	2.443
3800	19.720	101.888	84.808	64.907	-259.078	-35.485	2.041
3900	19.727	102.401	85.252	66.879	-259.153	-29.593	1.658
4000	19.734	102.900	85.687	68.852	-259.242	-23.708	1.295
4100	19.741	103.386	86.113	70.826	-259.346	-17.818	0.950
4200	19.747	103.864	86.5[illegible]0	72.800	-259.466	-11.921	0.620
4300	19.753	104.328	86.939	74.775	-259.604	-6.029	0.306
4400	19.758	104.782	87.339	76.751	-259.760	-0.126	0.006
4500	19.763	105.227	87.732	78.727	-259.933	5.769	-0.280
4600	19.768	105.561	88.117	80.704	-260.130	11.676	-0.555
4700	19.77[illegible]	106.086	88.494	82.681	-260.348	17.605	-0.819
4800	19.776	106.503	88.865	84.658	-260.592	23.513	-1.071
4900	19.780	106.910	89.229	86.636	-260.859	29.434	-1.313
5000	19.784	107.310	89.587	88.614	-261.154	35.365	-1.546
5100	19.787	107.702	89.938	90.593	-261.479	41.304	-1.770
5200	19.790	108.086	90.284	92.572	-261.834	46.313	-1.946
5300	19.793	108.463	90.623	94.551	-262.226	53.187	-2.193
5400	19.796	108.833	90.957	96.531	-262.652	59.150	-2.394
5500	19.799	109.196	91.285	98.510	-263.120	65.115	-2.587
5600	19.802	109.553	91.608	100.491	-263.630	71.088	-2.774
5700	19.804	109.904	91.926	102.471	-264.188	77.075	-2.955
5800	19.806	110.[illegible]	92.239	104.451	-264.802	83.076	-3.130
5900	19.8[illegible]	110.[illegible]	92.547	106.432	-265.476	89.077	-3.299
6000	19.8[illegible]	110.920	92.951	108.413	-266.216	95.106	-3.464

15 September 1962   RCF

DIMERIC BERYLLIUM OXIDE (Be_2O_2) (IDEAL MOLECULAR GAS) gfw= 50.026

ΔH°_{f0} = -101.691 Kcal gfw^{-1}

$\Delta H^\circ_{f298.15}$ = -107.700 kcal gfw^{-1}

Point Group = planar

$S^\circ_{298.15}$ = 58.562 cal deg K^{-1} gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 3.000 Kcal gfw^{-1}

Bond lengths and angles:

Be-O distance = 1.63 A

Heat of Formation

Third law calculations of the data of Chupka, et al[1] were made.

Heat Capacity and Entropy

Values of C_p°, S_t°, $(F-H^\circ_{298})/T$ and $H-H^\circ_{298}$ given by Hildenbrand[2] were used.

References

1. Chupka, W., et al. J. Chem. Phys. 30, 827 (1959).

2. Hildenbrand, D.L., Aeronutronic Publ. No. C-623, Contract NOrd 17980 (Sept. 1959).

TABLE 102

BERYLLIUM NITRIDE CONDENSED PHASE Be_3N_2

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Be from 0° to 1556°K, Liquid Be from 1556° to 2767°K, Gaseous Be from 2767° to 6000°K, Gaseous N_2. Solid Be_3N_2 from 0° to 2470°K, Liquid Be_3N_2 from 2470° to 3500°K.

T, °K	C_p° (cal/deg gfw)	S_T° (cal/deg gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/deg gfw)	$H_T^\circ - H_{298}^\circ$ (kcal/gfw)	ΔH_f° (kcal/gfw)	ΔF_f° (kcal/gfw)	Log K_p
0							
298.15	16.498	12.000	12.000	0.000	-132.000	-119.890	87.878
300	16.580	12.102	12.000	0.031	-132.003	-119.814	87.280
400	19.825	17.362	12.695	1.867	-132.184	-115.724	63.225
500	21.884	22.020	14.104	3.958	-132.305	-111.591	48.774
600	23.477	26.155	15.774	6.228	-132.380	-107.443	39.134
700	24.849	29.879	17.528	8.646	-132.405	-103.284	32.245
800	26.104	33.280	19.287	11.194	-132.388	-99.126	27.079
900	27.291	36.424	21.019	13.864	-132.332	-94.967	23.060
1000	28.435	39.358	22.707	16.651	-132.236	-90.822	19.848
1100	29.552	42.121	24.348	19.550	-132.114	-86.691	17.223
1200	30.650	44.740	25.939	22.561	-131.956	-82.572	15.038
1300	31.734	47.236	27.482	25.680	-131.763	-78.466	13.191
1400	32.809	49.627	28.979	28.907	-131.535	-74.376	11.610
1500	33.877	51.927	30.433	32.242	-131.273	-70.300	10.242
1556	34.472	53.180	31.229	34.155	-131.115	-68.028	9.554
1556	34.469	53.180	31.229	34.155	-141.675	-68.028	9.554
1600	34.936	54.147	31.846	35.682	- 41.425	-65.945	9.007
1700	35.994	56.297	33.221	39.229	-140.799	-61.245	7.873
1800	37.049	58.384	34.561	42.881	-140.090	-56.584	6.870
1900	38.101	60.415	35.869	46.638	-139.295	-51.966	5.977
2000	39.151	62.346	37.146	50.501	-138.414	-47.392	5.179
2100	40.199	64.332	38.395	54.468	-137.447	-42.856	4.460
2200	41.246	66.226	39.617	58.541	-136.393	-38.374	3.812
2300	42.291	68.083	40.814	62.717	-135.258	-33.942	3.225
2400	43.336	69.905	41.989	66.999	-134.046	-29.560	2.692
2470	44.067	71.161	42.798	70.058	-133.129	-26.537	2.348
2470	44.067	83.661	42.798	100.933	-102.254	-26.537	2.348
2500	44.067	84.193	43.291	102.255	-101.851	-25.605	2.238
2600	44.067	85.921	44.898	106.662	-100.537	-22.583	1.898
2700	44.067	87.584	46.448	111.068	-99.242	-19.610	1.587
2767.61	44.067	88.674	47.466	114.048	-98.383	-17.627	1.392
2767.61	44.067	88.674	47.466	114.048	-308.890	-17.627	1.392
2800	44.067	89.187	47.946	115.475	-308.229	-14.249	1.112
2900	44.067	90.733	49.395	119.882	-306.205	-3.782	0.285
3000	44.067	92.227	50.798	124.288	-304.186	6.618	-0.482
3100	44.067	93.672	52.15[illegible]	128.695	-30[illegible].173	16.946	-1.195
3200	44.067	95.071	53.477	133.102	-300.169	27.206	-1.858
3300	44.067	96.427	54.758	137.509	-29[illegible].141	37.398	-2.477
3400	44.067	97.743	56.30[illegible]	141.915	-296.152	47.540	-3.056
3500	44.067	99.020	57.2[illegible]4	146.322	-294.205	57.626	-3.598

15 September 1963 RED

BERYLLIUM NITRIDE (Be_3N_2) (CONDENSED PHASE) gfw = 55.055

$\Delta Hf^{\circ}_{298.15}$ = -132 ± 3 kcal gfw^{-1}

$S^{\circ}_{298.15}$ = 12 ± 2 cal deg^{-1} gfw^{-1}

T_m = 2470°K

ΔH_m = 30.875 ± 3.7 kcal gfw^{-1}

$C_p^{\circ} = 18.510 + 10.377 \times 10^{-3} T - 45.390 \times 10^{+4} T^{-2}$ cal deg K^{-1} gfw^{-1} 298°K ≤ T ≤ 2470°K

C_p° = 44.06 cal deg K^{-1} gfw^{-1} 2470°K ≤ T ≤ 3500°K

Structure

Body centered anti-Mn_2O_3 (D5) structure: a = 8.13 ± 0.10 kX.

Heat of Formation

Value obtained from NBS Report 6645[1] based on Neumann *et al*[2] direct nitriding.

Heat Capacity and Entropy

Low-temperature data was estimated by Kelley.[3] High-temperature data of Sato[4] and Kelley[5] was recalculated and extrapolated. Liquid heat capacity assumed equal to that of solid at m.p. and constant to 3500°K.

Melting and Vaporization

Melting point assumed at 2470°K based on Brewer[6] *et al*.

References

1. Beckett, C. W., *et al*, Prelim, Report, Selected Light Element Compds, NBSR 6645 (1960).
2. Neumann, B., C. Kroger, & H. Haebler, Z Anorg. U Allgem Chim. 204, 81 (1932).
3. Kelley, K. K., Bur of Mines Bulletin 407 (1937).
4. Sato, S., Sci Papers Inst. Phys. Chem. Research (Tokyo) 34, 888 (1938).
5. Kelley, K. K., U.S. Bureau of Mines Report 584 (1960).
6. Brewer, L., L. Bromley, P. Gilles, & N. Lofgren., The Chem & Met of Miscellaneous Materials., McGraw-Hill (1950).

BERYLLIUM NITRIDE (Be_3N_2) (CONDENSED PHASE) GFW = 55.055

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C_p° (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^{\circ}_T - H^{\circ}_{298})/T$ (cal/°K gfw)	$H^{\circ}_T - H^{\circ}_{298}$ (Kcal gfw)	ΔH_f (Kcal gfw)	ΔF_f (Kcal gfw)	log K_p
298.15	±0.826	±2.000	±2.000	±0.000	±3.000		
500	±1.094	±2.501	±2.105	±0.198			
1000	±1.421	±3.368	±2.535	±0.832			
1500	±1.693	±3.996	±2.922	±1.612			
1556	±1.723	±4.059	±2.961	±1.707			
1556	±2.757	±4.059	±2.961	±1.707			
2000	±3.132	±4.796	±3.289	±3.015			
2470	±3.525	±5.497	±3.643	±4.580			
2470	±5.000	±6.995	±3.643	±8.280			
2500	±5.000	±7.056	±3.684	±8.430			
3000	±5.000	±7.967	±4.324	±10.930			
3500	±5.000	±8.738	±4.901	±13.430			

TABLE 103

TRIMERIC BERYLLIUM OXIDE IDEAL MOLECULAR GAS **Be_3O_3**

Reference State for Calculating ΔH_f°, ΔF_f° and Log K_p: Solid Be from 0° to 1556°K, Liquid Be from 1556° to 2768°K, Gaseous Be from 2768° to 6000°K, Gaseous O_2, Gaseous Be_3O_3

T, °K	C_p (cal/°K gfw)	S_T (cal/°K gfw)	$-(F_T - H_{298})/T$ (cal/°K gfw)	$H_T - H_{298}$ (Kcal/gfw)	ΔH_f (Kcal/gfw)	ΔF_f (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-3.750	-251.936	-251.936	INFINITE
298.15	15.367	64.254	64.254	0.000	-252.700	-247.899	181.706
300	15.443	64.349	64.254	0.028	-252.713	-247.868	180.563
400	19.195	69.325	64.907	1.767	-253.359	-246.156	134.487
500	22.101	73.936	66.258	3.838	-253.893	-244.288	106.773
600	24.248	78.165	67.895	6.161	-254.336	-242.327	88.263
700	25.820	82.028	69.643	8.669	-254.710	-240.296	75.020
800	26.981	85.555	71.415	11.312	-255.052	-238.215	65.074
900	27.850	88.786	73.168	14.056	-255.383	-236.086	57.327
1000	28.513	91.756	74.880	16.875	-255.723	-233.925	51.122
1100	29.028	94.499	76.540	19.753	-256.092	-231.731	46.039
1200	29.434	97.042	78.144	22.677	-256.492	-229.503	41.796
1300	29.758	99.412	79.690	25.637	-256.933	-227.240	38.201
1400	30.022	101.627	81.179	28.627	-257.417	-224.941	35.113
1500	30.238	103.706	82.612	31.640	-257.953	-222.599	32.431
1556	30.341	104.814	83.387	33.341	-258.275	-221.264	31.076
1556	30.341	104.814	83.387	33.341	-268.877	-221.264	31.076
1600	30.418	105.663	83.992	34.673	-269.033	-219.925	30.039
1700	30.568	107.512	85.322	37.723	-26 .387	-216.845	27.876
1800	30.696	109.263	86.604	40.786	-269.751	-213.747	25.951
1900	30.805	110.926	87.840	43.862	-270.125	-210.625	24.226
2000	30.898	112.508	89.035	46.947	-270.514	-207.486	22.672
2100	30.979	114.018	90.189	50.041	-270.918	-204.319	21.263
2200	31.050	115.461	91.305	53.143	-271.337	-201.138	19.980
2300	31.112	116.842	92.385	56.251	-271.775	-197.938	18.808
2400	31.167	118.168	93.432	59.365	-272.228	-194.715	17.730
2500	31.215	119.441	94.447	62.484	-272.703	-191.476	16.738
2600	31.258	120.666	95.432	65.608	-273.194	-188.219	15.820
2700	31.296	121.847	96.389	68.736	-273.705	-184.945	14.970
2767.61	31.321	122.624	97.022	70.865	-274.063	-182.703	14.425
2767.61	31.321	122.624	97.022	70.865	-484.528	-182.703	14.425
2800	31.331	122.985	97.318	71.867	-484.458	-179.211	13.987
2900	31.362	124.085	98.223	75.002	-484.246	-168.314	12.684
3000	31.390	125.149	99.102	78.139	-484.040	-157.413	11.467
3100	31.415	126.179	99.959	81.280	-483.843	-146.523	10.329
3200	31.438	127.177	100.794	84.422	-483.659	-135.652	9.264
3300	31.460	128.144	101.609	87.567	-483.483	-124.789	8.264
3400	31.479	129.084	102.403	90.714	[illegible]	-113.917	7.322
3500	31.496	129.997	103.178	93.864	[illegible]	-103.045	6.434
3600	31.513	130.884	103.936	97.014	-483.033	-92.199	5.597
3700	31.528	131.748	104.676	100.166	-482.909	-81.338	4.804
3800	31.541	132.589	105.399	103.319	-492.809	-70.488	4.054
3900	31.554	133.408	106.107	106.474	-482.724	-59.632	3.342
4000	31.566	134.207	106.900	109.630	-482.661	-48.790	2.666
4100	31.577	134.987	107.478	112.787	-482.621	-37.942	2.022
4200	31.587	135.748	108.142	115.946	-482.603	-27.089	1.410
4300	31.597	136.491	108.792	119.105	-482.613	-16.243	0.826
4400	31.606	137.218	109.430	122.265	-482.652	-5.394	0.268
4500	31.614	137.928	110.056	125.426	[illegible]	5.442	-0.264
4600	31.622	138.623	110.669	128.588	-482.813	16.294	-0.774
4700	31.629	139.303	111.271	131.751	-482.943	27.166	-1.263
4800	31.636	139.969	111.862	134.914	[illegible]	38.010	-1.731
4900	31.642	[illegible]	112.442	138.078	-483.314	48.869	-2.180
5000	31.648	[illegible]	113.012	141.242	-483.560	59.740	-2.611
5100	31.654	141.888	113.572	144.407	-483.851	70.614	-3.026
5200	31.659	142.502	114.123	147.573	-484.186	80.095	-3.366
5300	31.664	143.106	114.664	150.739	-484.577	92.364	-3.809
5400	31.669	143.697	115.196	153.906	-485.018	103.268	-4.179
5500	31.674	144.279	115.720	157.073	-485.522	114.164	-4.536
5600	31.678	144.849	116.235	160.241	-486.091	125.073	-4.881
5700	31.682	145.410	116.742	163.409	-486.730	136.000	-5.214
5800	31.686	145.961	117.241	166.578	-487.452	146.946	-5.537
5900	[illegible]	146.503	117.732	169.746	-488.266	157.887	-5.848
6000	[illegible]	147.036	118.216	172.916	-489.177	168.877	-6.151

15 September 1962 RCF

TRIMERIC BERYLLIUM OXIDE (Be_3O_3) (IDEAL MOLECULAR GAS) gfw = 75.039

ΔH°_{f0} = -251.936 Kcal gfw^{-1}

$\Delta H^\circ_{f298.15}$ = -252.700 ± kcal gfw^{-1}

Point Group = planar

$S^\circ_{298.15}$ = 64.254 cal degK^{-1}gfw^{-1}

$H^\circ_{298.15}-H^\circ_0$ = 3.750 Kcal gfw^{-1}

Bond lengths and angles:

Be-O distance = 1.63 A

Heat of Formation

Third law calculations of data by Chupka, *et al*[1] were made.

Heat Capacity and Entropy

Values given by Hildenbrand[2] were used.

References

1. Chupka, W., *et al*, J. Chem. Phys. 30, 827 (1959).
2. Hildenbrand, D. L., Aeronutronic Publ. No. C-623, Contract NOrd 17980 (1959).

TABLE 104

TETRAMERIC BERYLLIUM OXIDE IDEAL MOLECULAR GAS Be_4O_4

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Be from 0° to 1556°K, Liquid Be from 1556° to 2768°K, Gaseous Be from 2768° to 6000°K, Gaseous O_2, Gaseous Be_4O_4

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-4.500	-376.082	-376.082	INFINITE
298.15	21.520	72.309	72.309	0.000	-377.600	-367.215	269.163
300	21.625	72.442	72.310	0.039	-377.615	-367.149	267.455
400	26.751	79.393	73.222	2.468	-378.366	-363.546	198.623
500	30.685	85.507	75.107	5.349	-378.959	-359.766	157.246
600	33.581	91.671	77.387	8.570	-379.426	-355.885	129.625
700	36.696	97.015	79.815	12.040	-379.798	-351.932	109.873
800	37.257	101.889	82.274	15.691	-380.127	-347.930	95.045
900	38.425	106.348	84.705	19.478	-380.440	-343.882	83.502
1000	39.316	110.444	87.077	23.367	-380.763	-339.803	74.260
1100	40.006	114.225	89.375	27.335	-381.125	-335.696	66.693
1200	40.551	117.730	91.594	31.364	-381.528	-331.554	60.381
1300	40.986	120.994	93.731	35.441	-381.985	-327.375	55.034
1400	41.340	124.045	95.789	39.558	-382.500	-323.158	50.445
1500	41.630	126.907	97.769	43.707	-383.083	-318.895	46.461
1556	41.765	128.430	98.839	46.044	-383.444	-316.479	44.449
1556	41.765	128.430	98.839	46.044	-397.580	-316.479	44.449
1600	41.871	129.602	99.675	47.883	-397.725	-314.197	42.915
1700	42.073	132.147	101.511	52.080	-398.066	-308.966	39.718
1800	42.244	134.557	103.281	56.296	-398.420	-303.719	36.875
1900	42.390	136.845	104.987	60.528	-398.788	-298.448	34.328
2000	42.516	139.022	106.635	64.774	-399.174	-293.158	32.033
2100	42.625	141.099	108.227	69.031	-399.581	-287.840	29.954
2200	42.719	143.085	109.767	73.298	-400.008	-282.509	28.063
2300	42.803	144.985	111.257	77.575	-400.459	-277.161	26.335
2400	42.876	146.809	112.701	81.859	-400.931	-271.786	24.748
2500	42.941	148.560	114.100	86.150	-401.432	-266.395	23.287
2600	42.998	150.246	115.458	90.447	-401.955	-260.985	21.937
2700	43.050	151.869	116.777	94.749	-402.505	-255.557	20.685
2767.61	43.081	152.938	117.650	97.678	-402.892	-251.850	19.884
2767.61	43.081	152.938	117.650	97.678	-683.512	-251.850	19.884
2800	43.096	153.436	118.058	99.056	-683.378	-246.857	19.267
2900	43.138	154.949	119.305	103.368	-682.962	-231.275	17.428
3000	43.175	156.412	120.517	107.684	-682.554	-215.693	15.712
3100	43.209	157.628	121.698	112.003	-682.161	-200.131	14.109
3200	43.240	159.201	122.849	116.326	-681.782	-184.598	12.607
3300	43.269	160.532	123.970	120.651	-681.415	-169.073	11.197
3400	43.294	161.824	125.06[illegible]	124.979	-68[illegible] 063	-153.550	9.870
3500	43.318	163.079	126.13[illegible]	129.310	-68[illegible] 732	-138.028	8.618
3600	43.340	164.300	127.177	133.643	-680.419	-122.544	7.439
3700	43.360	165.487	128.196	137.978	-680.122	-107.041	6.322
3800	43.378	166.644	129.193	142.315	-679.855	-91.563	5.266
3900	43.395	167.771	130.167	146.654	-679.610	-76.072	4.263
4000	43.411	168.820	131.121	150.994	-679.394	-60.604	3.311
4100	43.426	169.[illegible]2	132.055	155.336	-679.208	-45.135	2.406
4200	43.440	170.989	132.970	159.680	-679.052	-29.664	1.543
4300	43.453	172.011	133.866	164.024	-678.934	-14.207	0.722
4400	43.464	173.010	134.744	168.370	-678.852	1.258	-0.062
4500	43.476	173.987	135.605	172.717	-678.803	16.704	-0.811
4600	43.486	174.943	136.450	177.065	-678.803	32.159	-1.528
4700	43.496	175.878	137.279	181.415	-678.843	47.642	-2.215
4800	43.505	176.794	138.093	185.765	-678.935	63.083	-2.872
4900	43.514	177.691	138.892	190.116	-679.074	78.541	-3.503
5000	43.522	178.570	139.[illegible]	194.467	-679.2[illegible]	94.015	-4.109
5100	43.529	179.432	140.448	198.820	-679.524	109.491	-4.692
5200	43.536	180.278	141.206	203.173	-679.839	123.108	-5.174
5300	43.54[illegible]	181.107	141.[illegible]51	207.527	-680.227	140.438	-5.791
5400	43.550	181.921	142.683	211.882	-680.684	155.947	-6.311
5500	43.[illegible]	182.720	143.404	216.237	-681.223	171.443	-6.812
5600	43.56[illegible]	183.505	144.113	220.593	-681.849	186.953	-7.296
5700	43.567	184.276	144.811	224.950	-682.568	202.483	-7.763
5800	43.572	185.034	145.498	229.307	-683.399	218.037	-8.215
5900	43.577	185.779	146.174	233.664	-684.352	233.581	-8.652
6000	43.582	186.511	146.841	238.022	-685.436	249.178	-9.076

15 September 1962 RCF

TETRAMERIC BERYLLIUM OXIDE (Be_4O_4) (IDEAL MOLECULAR GAS) gfw = 100.052

$\Delta H^\circ_{f0} = -376.082$ Kcal gfw^{-1}

$\Delta H^\circ_{f298.15} = -377.600 \pm 4.000$ Kcal gfw^{-1}

Point Group = planar

$S^\circ_{298.15} = 72.309$ cal degK^{-1}gfw^{-1}

$H^\circ_{298.15} - H^\circ_0 = 4.500$ Kcal gfw^{-1}

Bond lengths and angles:

Be-O distance = 1.63 A

Heat of Formation

Based on data of Chupka *et al*[1].

Heat Capacity and Entropy

Values given by Hildenbrand[2] were used.

References

1. Chupka, W., *et al*, J. Chem. Phys. 30, 827 (1959).
2. Hildenbrand, D. L., Aeronutronic Publ. No. C-623, Contract NOrd 17980 (1959).

TABLE 105

PENTAMERIC BERYLLIUM OXIDE IDEAL MOLECULAR GAS **Be_5O_5**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p Solid Be from 0° to 1556°K, Liquid Be from 1556° to 2768°K, Gaseous Be from 2768° to 6000°K, Gaseous O_2, Gaseous Be_5O_5

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-5.250	-500.227	-500.227	INFINITE
298.15	27.673	79.700	79.700	0.000	-502.500	-486.332	356.474
300	27.806	79.871	79.701	0.051	-502.517	-486.231	354.202
400	34.307	88.798	80.873	3.169	-503.374	-480.671	262.614
500	39.269	97.013	83.292	6.860	-504.025	-474.911	207.573
600	42.913	104.513	86.214	10.979	-504.516	-469.045	170.841
700	45.573	111.338	89.323	15.410	-504.888	-463.103	144.580
800	47.532	117.558	92.469	20.070	-505.202	-457.113	124.872
900	49.000	123.245	95.578	24.901	-505.497	-451.079	109.532
1000	50.118	128.469	98.609	29.859	-505.804	-445.017	97.254
1100	50.985	133.288	101.546	34.916	-506.159	-438.929	87.203
1200	51.668	137.754	104.379	40.050	-506.565	-432.806	78.821
1300	52.215	141.912	107.108	45.245	-507.038	-426.646	71.722
1400	52.658	145.799	109.735	50.489	-507.584	-420.446	65.631
1500	52.022	149.445	112.262	55.774	-508.214	-414.194	60.345
1556	53.196	151.383	113.626	58.750	-508.610	-410.659	57.677
1556	53.196	151.383	113.626	58.750	-526.280	-410.659	57.677
1600	53.325	152.877	114.694	61.092	-526.418	-407.406	55.646
1700	53.578	156.117	117.036	66.437	-526.[illegible]45	-399.958	51.416
1800	53.793	159.186	119.293	71.806	-527.089	-392.494	47.653
1900	53.976	162.099	121.470	77.195	-527.450	-385.009	44.284
2000	54.134	164.872	123.572	82.601	-527.834	-377.504	41.250
2100	54.270	167.517	125.602	88.021	-528.244	-369.968	38.501
2200	54.389	170.044	127.565	93.454	-528.679	-362.421	36.001
2300	54.493	172.464	129.465	98.898	-529.145	-354.857	33.718
2400	54.585	174.785	131.305	104.353	-529.635	-347.262	31.621
2500	54.666	177.015	133.089	109.815	-530.162	-339.654	29.691
2600	54.738	179.161	134.820	115.286	-530.717	-332.025	27.908
2700	54.803	181.228	136.501	120.763	-531.305	-324.377	26.255
2767.61	54.843	182.588	137.613	124.491	-531.722	-319.156	25.198
2767.61	54.843	182.588	137.613	124.491	-882.496	-319.156	25.198
2800	54.861	183.222	138.134	126.246	-882.297	-312.643	24.402
2900	54.913	185.148	139.722	131.735	-881.678	-292.307	22.028
3000	54.960	187.011	141.268	137.229	-881.069	-271.982	19.813
3100	55.003	188.814	142.773	142.727	-880.478	-251.681	17.743
3200	55.042	190.[illegible]60	144.239	148.229	-879.906	-231.417	15.804
3300	55.078	192.255	145.668	153.735	-879.[illegible]48	-211.169	13.984
3400	55.110	193.900	147.063	[illegible]9.245	-878.[illegible]	-190.926	12.272
3500	55.14[illegible]	195.497	148.424	164.757	-878.[illegible]	-170.688	10.658
3600	55.167	197.051	149.753	170.273	-877.80[illegible]	-150.494	9.136
3700	55.192	198.563	151.052	175.791	-877.334	-130.287	7.695
3800	55.215	200.035	152.322	181.311	-87[illegible].902	-110.110	6.332
3900	55.237	2[illegible].470	153.564	186.834	-876.496	-89.925	5.039
4000	55.257	202.869	154.779	192.358	-876.127	-69.766	3.812
4100	55.275	204.233	155.968	197.885	-875.795	-49.606	2.644
4200	55.292	205.565	157.134	203.414	-875.501	-29.450	1.532
4300	55.308	206.867	158.275	208.944	-875.253	-9.312	0.473
4400	55.323	208.138	159.394	214.475	-875.053	10.830	-0.538
4500	55.337	209.382	160.491	220.008	-874.892	30.948	-1.503
4600	55.350	210.598	161.567	225.543	-874.792	51.078	-2.427
4700	55.363	211.789	162.623	231.078	-874.744	71.238	-3.312
4800	55.374	212.954	163.660	236.615	-874.760	91.344	-4.159
4900	55.385	214.096	164.677	242.153	-874.835	111.472	-4.972
5000	55.395	215.215	165.677	247.692	-874.978	131.615	-5.753
5100	55.405	216.312	166.659	253.232	-875.198	151.759	-6.503
5200	55.414	217.388	167.624	258.773	-875.492	169.579	-7.127
5300	55.422	218.444	168.573	264.315	-875.878	192.036	-7.918
5400	55.430	219.480	169.506	269.858	-876.349	212.217	-8.588
5500	55.438	220.497	170.424	275.401	-876.924	232.374	-9.233
5600	55.445	221.496	171.327	280.945	-877.607	252.551	-9.856
5700	55.452	222.478	172.216	286.490	-878.407	272.751	-10.457
5800	55.458	223.442	173.091	292.036	-879.346	292.979	-11.039
5900	55.465	224.390	173.952	297.582	-880.438	313.193	-11.601
6000	55.470	225.322	174.801	303.129	-881.693	333.474	-12.146

15 September 1962 RCF

PENTAMERIC BERYLLIUM OXIDE (Be_5O_5)(IDEAL MOLECULAR GAS) gfw = 125.065

$\Delta H^\circ_{f0} = -500.227$ Kcal gfw $^{-1}$

$\Delta H^\circ_{f298.15} = -502.$ Kcal gfw^{-1}

Point Group = planar

$S^\circ_{298.15} = 79.700$ cal degK^{-1}gfw^{-1}

$H^\circ_{298.15} - H^\circ_0 = 5.250$ Kcal gfw^{-1}

Bond lengths and angles:

Be-O distance = 1.63 A .

Heat of Formation

Based on data of Chupka et al.[1]

Heat Capacity and Entropy

Values given by Hildenbrand[2] were used.

References

1. Chupka, W., et al, J. Chem. Phys. 30, 827 (1959).

2 Hildenbrand, D. L., Aeronutronic Publ. No. C-623, Contract NOrd 17980 (1959).

TABLE 106

HEXAMERIC BERYLLIUM OXIDE IDEAL MOLECULAR GAS Be_6O_6

Reference State for Calculating ΔH_f°, ΔF_f° and Log K_p: Solid Be from 0° to 1556°K, Liquid Be from 1556° to 2768°K, Gaseous Be from 2768° to 6000°K, Gaseous O_2, Gaseous Be_6O_6

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-6.000	-629.773	-629.773	INFINITE
298.15	33.825	86.687	86.687	0.000	-632.800	-610.729	447.655
300	33.988	86.896	86.688	0.062	-632.819	-610.591	444.794
400	41.864	97.798	86.121	3.870	-633.781	-603.035	329.467
500	47.853	107.817	91.073	8.371	-634.491	-595.255	260.173
600	52.246	116.951	94.637	13.388	-635.006	-587.362	213.936
700	55.449	125.258	98.427	18.781	-635.376	-579.391	180.885
800	57.808	132.824	102.261	24.450	-635.677	-571.374	156.085
900	59.574	139.740	106.047	30.323	-635.954	-563.313	136.784
1000	60.920	146.089	109.738	36.351	-636.244	-555.227	121.339
1100	61.963	151.946	113.312	42.497	-636.593	-547.118	108.697
1200	62.785	157.375	116.761	48.736	-637.002	-538.974	98.156
1300	63.443	162.427	120.082	55.049	-637.490	-530.793	89.230
1400	63.976	167.149	123.277	61.421	-638.066	-522.568	81.573
1500	64.414	171.578	126.351	67.841	-638.744	-514.288	74.928
1556	64.622	173.932	128.009	71.456	-639.176	-509.610	71.574
1556	64.622	173.932	128.009	71.456	-660.296	-509.610	71.574
1600	64.778	175.747	129.309	74.301	-660.427	-505.370	69.027
1700	65.083	179.684	132.158	80.795	-660.740	-495.664	63.719
1800	65.341	183.412	134.902	87.316	-661.074	-485.943	58.999
1900	65.562	186.951	137.549	93.862	-661.428	-476.202	54.773
2000	65.751	190.318	140.104	100.428	-661.810	-466.440	50.968
2100	65.915	193.550	142.573	107.011	-662.223	-456.648	47.522
2200	66.058	196.670	144.959	113.610	-662.665	-446.843	44.388
2300	66.183	199.539	147.269	120.222	-663.145	-437.024	41.525
2400	66.294	202.359	149.506	126.846	-663.655	-427.170	38.897
2500	66.392	205.067	151.674	133.481	-664.208	-417.303	36.479
2600	66.479	207.673	153.778	140.124	-664.795	-407.414	34.245
2700	66.556	210.183	155.821	146.776	-665.421	-397.506	32.174
2767.61	66.604	211.834	157.172	151.305	-665.866	-390.744	30.850
2767.61	66.604	211.834	157.172	151.305	-1086.880	-390.744	30.850
2800	66.626	212.605	157.806	153.436	-1086.615	-382.698	29.870
2900	66.689	214.944	159.736	160.101	-1085.794	-357.570	26.946
3000	66.746	217.206	161.615	166.773	-1084.984	-332.458	24.218
3100	66.797	219.395	163.443	173.450	-1084.196	-307.374	21.669
3200	66.844	221.517	165.225	180.133	-1083.429	-282.342	19.282
3300	66.887	223.574	166.962	186.819	-1082.680	-257.333	17.042
3400	66.925	225.572	168.657	193.510	-1081.953	-232.328	14.933
3500	66.961	227.512	170.311	200.204	-1081.259	-207.333	12.946
3600	66.994	229.399	171.926	206.902	-1080.591	-182.393	11.072
3700	67.024	231.235	173.504	213.603	-1079.947	-157.439	9.299
3800	67.052	233.023	175.047	220.307	-1079.348	-132.522	7.621
3900	67.078	234.765	176.556	227.014	-1078.782	-107.599	6.029
4000	67.102	236.463	178.033	233.723	-1078.259	-82.712	4.519
4100	67.124	238.121	179.478	240.434	-1077.782	-57.824	3.082
4200	67.145	239.738	180.894	247.147	-1077.351	-32.939	1.714
4300	67.164	241.319	182.281	253.863	-1076.974	-8.083	0.411
4400	67.182	242.863	183.640	260.580	-1076.653	16.781	-0.833
4500	67.199	244.373	184.973	267.299	-1076.381	41.610	-2.021
4600	67.215	245.850	186.280	274.020	-1076.182	66.455	-3.157
4700	67.229	247.296	187.563	280.742	-1076.045	91.334	-4.247
4800	67.243	248.711	188.822	287.466	-1075.984	116.149	-5.288
4900	67.256	250.098	190.059	294.191	-1075.994	140.979	-6.288
5000	67.268	251.457	191.273	300.917	-1076.087	165.835	-7.248
5100	67.280	252.789	192.46[illegible]	307.645	-1076.271	190.687	-8.171
5200	67.291	254.056	193.639	314.373	-1076.545	212.746	-8.941
5300	67.301	255.377	194.792	321.103	-1076.928	240.370	-9.911
5400	67.311	256.636	195.926	327.834	-1077.415	265.252	-10.735
5500	67.320	257.871	197.041	334.565	-1078.025	290.122	-11.528
5600	67.329	259.084	198.138	341.298	-1078.765	315.006	-12.293
5700	67.337	260.276	199.219	348.031	-1079.646	339.916	-13.032
5800	67.345	261.447	200.280	354.765	-1080.694	364.864	-13.748
5900	67.352	262.598	201.327	361.500	-1081.924	389.782	-14.438
6000	67.359	263.730	202.357	368.236	-1083.351	414.794	-15.108

15 September 1962 RCF

HEXAMERIC BERYLLIUM OXIDE (Be_6O_6) (IDEAL MOLECULAR GAS) gfw=150.078

ΔH°_{f0} = -629.773 Kcal gfw^{-1}

$\Delta H^\circ_{f298.15}$ = -632.800± 40.000 Kcalgfw^{-1}

Point Group = planar

$S^\circ_{298.15}$ = 86.687 cal degK^{-1}gfw^{-1}

$H^\circ_{298.15}-H^\circ_0$ = 6.000 Kcal gfw^{-1}

Bond lengths and angles:

Be-O distance = 1.63 A

Heat of Formation

Based on data of Chupka *et al*[1].

Heat Capacity and Entropy

Values given by Hildenbrand[2] were used.

References

1. Chupka, W., *et al*, J. Chem. Phys. 30, 827 (1959).

2. Hildenbrand, D. L., Aeronutronic Publ. No. C-623, Contract NOrd 17980 (1959).

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p
Solid Graphite from 0° to 6000°K

	cal/°K gfw			Kcal gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	0.252			
298.15	2.038	1.359	1.359	0.000			
300	2.054	1.372	1.359	0.004			
400	2.851	2.075	1.450	0.250			
500	3.496	2.784	1.646	0.569			
600	4.038	3.471	1.893	0.947			
700	4.440	4.126	2.166	1.372			
800	4.740	4.739	2.449	1.831			
900	4.970	5.311	2.736	2.318			
1000	5.149	5.844	3.020	2.824			
1100	5.304	6.342	3.300	3.347			
1200	5.430	6.809	3.573	3.883			
1300	5.527	7.248	3.839	4.432			
1400	5.605	7.661	4.098	4.988			
1500	5.669	8.050	4.348	5.552			
1600	5.721	8.417	4.591	6.122			
1700	5.765	8.765	4.827	6.696			
1800	5.803	9.096	5.055	7.275			
1900	5.836	9.411	5.276	7.857			
2000	5.865	9.711	5.490	8.442			
2100	5.891	9.998	5.698	9.029			
2200	5.914	10.272	5.900	9.620			
2300	5.936	10.536	6.095	10.212			
2400	5.956	10.789	6.286	10.807			
2500	5.974	11.032	6.471	11.403			
2600	5.992	11.267	6.651	12.002			
2700	6.009	11.492	6.826	12.602			
2800	6.026	11.712	6.997	13.203			
2900	6.042	11.924	7.163	13.807			
3000	6.057	12.129	7.325	14.412			
3100	6.073	12.328	7.483	15.018			
3200	6.088	12.521	7.638	15.626			
3300	6.103	12.708	7.788	16.236			
3400	6.119	12.891	7.936	16.847			
3500	6.134	13.068	8.080	17.460			
3600	6.150	13.241	8.221	18.074			
3700	6.165	13.410	8.35	18.690			
3800	6.181	13.575	8.494	19.307			
3900	6.197	13.736	8.626	19.926			
4000	6.213	13.693	8.755	20.546			
4100	6.230	14.046	8.883	21.168			
4200	6.247	14.197	9.008	21.792			
4300	6.264	14.344	9.130	22.418			
4400	6.281	14.488	9.250	23.045			
4500	6.299	14.629	9.368	23.674			
4600	6.317	14.768	9.484	24.305			
4700	6.335	14.904	9.598	24.937			
4800	6.354	15.038	9.710	25.572			
4900	6.373	15.169	9.820	26.208			
5000	6.392	15.298	9.928	26.846			
5100	6.412	15.424	10.035	27.487			
5200	6.432	15.549	10.140	28.129			
5300	6.452	15.672	10.243	28.773			
5400	6.473	15.793	10.34	29.419			
5500	6.494	15.912	10.445	30.068			
5600	6.516	16.029	10.543	30.718			
5700	6.538	16.144	10.641	31.371			
5800	6.560	16.258	10.737	32.026			
5900	6.583	16.371	10.831	32.683			
6000	6.606	16.481	10.924	33.342			

15 September 1962 CHW

CARBON (C) (REFERENCE STATE) gfw = 12.011

0°K to 6000 °K Crystal

$\Delta H^\circ_{f0} = 0$ $\Delta H^\circ_{f298.15} = 0$

$\Delta H^\circ_{s298.15} = 170.890$ Kcal gfw^{-1} $S^\circ_{298.15} = 1.359$ cal $deg K^{-1}$ gfw^{-1}

$H^\circ_{298.15} - H^\circ_0 = 0.252$ Kcal gfw^{-1}

Structure

The graphite structure is used as the reference state.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Data from JANAF tables were used in this table.

Reference

1. JANAF Thermochemical Tables, Dow Chemical Co.(31 December 1960).

CARBON

IDEAL MONATOMIC GAS

C

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p
Solid Graphite from 0° to 6000°K

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.562	169.580	169.580	INFINITE
298.15	4.981	37.761	37.761	0.000	170.890	160.037	-117.304
300	4.981	37.792	37.761	0.009	170.895	159.969	-116.532
400	4.975	39.224	37.957	0.507	171.147	156.287	-85.387
500	4.973	40.334	38.325	1.004	171.325	152.550	-66.677
600	4.971	41.240	38.738	1.502	171.445	148.783	-54.192
700	4.970	42.007	39.152	1.999	171.517	145.000	-45.269
800	4.970	42.670	39.551	2.496	171.555	141.209	-38.575
900	4.970	43.256	39.931	2.993	171.565	137.415	-33.367
1000	4.969	43.779	40.290	3.490	171.556	133.620	-29.201
1100	4.969	44.253	40.629	3.986	171.529	129.828	-25.793
1200	4.970	44.685	40.949	4.483	171.490	126.039	-22.954
1300	4.971	45.083	41.252	4.980	171.438	122.253	-20.552
1400	4.972	45.452	41.539	5.478	171.380	118.473	-18.494
1500	4.975	45.795	41.811	5.975	171.313	114.695	-16.710
1600	4.978	46.116	42.071	6.473	171.241	110.923	-15.151
1700	4.984	46.418	42.317	6.971	171.165	107.156	-13.775
1800	4.990	46.703	42.553	7.469	[illegible]	103.393	-12.553
1900	4.998	46.973	42.779	7.969	171.002	99.653	-11.460
2000	5.008	47.229	42.995	8.469	170.917	95.880	-10.477
2100	5.019	47.474	43.202	8.970	170.831	92.131	-9.588
2200	5.032	47.708	43.402	9.473	170.743	88.386	-8.780
2300	5.046	47.932	43.594	9.977	170.655	84.642	-8.042
2400	5.061	48.147	43.779	10.482	170.565	80.906	-7.367
2500	5.077	48.354	43.958	10.989	170.476	77.172	-6.746
2600	5.094	48.553	44.131	11.497	170.385	73.442	-6.173
2700	5.112	48.746	44.298	12.008	170.296	69.714	-5.643
2800	5.130	[illegible]	44.461	12.520	170.207	65.992	-5.151
2900	5.149	[illegible]	44.618	13.034	170.117	62.271	-4.693
3000	5.168	49.287	44.771	13.550	170.028	58.553	-4.265
3100	5.187	49.457	44.919	14.067	169.939	54.838	-3.866
3200	5.206	49.622	45.064	14.587	169.851	51.128	-3.492
3300	5.224	49.782	45.204	15.108	169.762	47.417	-3.140
3400	5.243	49.939	45.341	15.632	169.675	43.713	-2.810
3500	5.261	50.091	45.475	16.157	169.587	40.009	-2.498
3600	5.279	50.239	45.605	16.684	[illegible]	36.308	-2.204
3700	5.296	50.384	45.732	17.213	[illegible]	32.609	-1.926
3800	5.313	50.526	45.856	17.743	169.376	28.913	-1.663
3900	5.329	50.664	45.978	18.275	169.239	25.217	-1.413
4000	5.345	50.799	46.097	18.809	169.153	21.527	-1.176
4100	5.360	50.931	46.213	19.344	169.066	17.837	-0.950
4200	5.375	51.061	46.327	19.881	168.979	14.150	-0.736
4300	5.388	51.187	46.439	20.419	168.891	10.463	-0.531
4400	5.402	51.311	46.548	20.959	168.804	6.779	-0.336
4500	5.414	51.433	46.655	21.499	168.715	3.098	-0.150
4600	5.426	51.552	46.760	22.042	168.627	-0.580	0.027
4700	5.437	51.669	46.863	22.585	168.538	-4.258	0.198
4800	5.448	51.783	46.965	23.129	168.447	-7.933	0.361
4900	5.459	51.896	47.064	23.674	168.356	-11.607	0.517
5000	5.468	52.006	47.162	24.221	168.265	-15.280	0.667
5100	5.477	52.115	47.258	24.768	168.171	-18.948	0.811
5200	5.486	52.221	47.352	25.316	168.077	-22.615	0.950
5300	5.494	52.326	47.445	25.865	167.982	-26.282	1.084
5400	5.502	52.428	47.537	26.415	167.886	-29.945	1.212
5500	5.509	52.529	47.627	26.966	167.788	-33.608	1.335
5600	5.516	52.629	47.715	27.517	167.689	-37.273	1.455
5700	5.523	52.726	47.802	28.069	167.588	-40.928	1.569
5800	5.529	52.822	47.888	28.621	167.485	-44.584	1.680
5900	5.535	52.917	47.972	29.175	167.382	-48.243	1.787
6000	5.541	53.010	48.055	29.728	167.276	-51.898	1.890

15 September 1962 CHW

CARBON, MONATOMIC (C) (IDEAL GAS)

gfw = 12.011

ΔH°_{f0} = 169.580 Kcal gfw^{-1}

$\Delta H^\circ_{f298.15}$ = 170.890 Kcal gfw^{-1}

Ground State Configuration $^3P_0$

$S^\circ_{298.15}$ = 37.761 cal degK^{-1} gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 1.562 Kcal gfw^{-1}

Electronic levels and multiplicities

Source of Data

Atomic energy levels from Moore[1].

Heat of Formation

Value consistent with JANAF[2] was chosen.

Heat Capacity and Entropy

Calculated on monatomic gas computer program.

References

1. Moore, C., Atomic Energy Levels, Vol.1, Nat'l. Bur. Stds. (1949).
2. JANAF Thermochemical Tables, Dow Chemical Co. (1960).

CARBON, MONATOMIC (C) (IDEAL GAS) GFW = 12.011

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T - H_{298})/T$ (cal/°K gfw)	$H_T - H_{298}$ (Kcal/gfw)	ΔH_f (Kcal/gfw)	ΔF_f (Kcal/gfw)	log K_f
± 298.15	± 0.000	± 0.002	± 0.002	± 0.000	± 0.450		
± 1000	± 0.000	± 0.002	± 0.002	± 0.000			
± 2000	± 0.000	± 0.002	± 0.002	± 0.000			
± 3000	± 0.000	± 0.002	± 0.002	± 0.001			
± 4000	± 0.000	± 0.002	± 0.002	± 0.001			
± 5000	± 0.000	± 0.002	± 0.003	± 0.001			
± 6000	± 0.000	± 0.002	± 0.003	± 0.001			

TABLE 109

HAFNIUM CARBIDE **CONDENSED PHASE** **CHf**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Hf from 0° to 2495°K, Liquid Hf from 2495° to 4985°K, Gaseous Hf from 4985° to 6000°K; Solid C, Solid HfC from 0° to 3900°K

T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
	cal/°K gfw			Kcal/gfw			
0	0.000	0.000	INFINITE	-1.494	-54.807	-54.807	INFINITE
298.15	8.228	9.852	9.852	0.000	-55.000	-54.339	39.830
300	8.274	9.903	9.852	0.015	-55.001	-54.335	39.581
400	9.916	12.539	10.200	0.936	-54.990	-54.114	29.565
500	10.746	14.850	10.905	1.973	-54.974	-53.899	23.558
600	11.256	16.857	11.733	3.074	-54.976	-53.686	19.554
700	11.615	18.621	12.594	4.219	-54.998	-53.470	16.693
800	11.894	20.191	13.447	5.395	-55.039	-53.248	14.546
900	12.126	21.605	14.276	6.596	-55.101	-53.020	12.874
1000	12.329	22.894	15.075	7.819	-55.177	-52.786	11.536
1100	12.513	24.078	15.840	9.061	-55.267	-52.543	10.439
1200	12.684	25.174	16.573	10.321	-55.369	-52.290	9.523
1300	12.846	26.195	17.274	11.598	-55.486	-52.028	8.746
1400	13.002	27.153	17.946	12.890	-55.610	-51.758	8.079
1500	13.152	28.055	18.590	14.198	-55.743	-51.478	7.500
1600	13.299	28.909	19.209	15.521	-55.885	-51.190	6.992
1700	13.443	29.719	19.803	16.858	-56.033	-50.889	6.542
1800	13.584	30.492	20.376	18.209	-56.189	-50.585	6.142
1900	13.724	31.230	20.928	19.575	-56.351	-50.269	5.782
2000	13.863	31.938	21.461	20.954	-56.519	-49.944	5.457
2033	13.908	32.165	21.633	21.412	-56.375	-49.836	5.357
2033	13.908	32.165	21.633	21.412	-58.225	-49.836	5.357
2100	14.000	32.617	21.976	22.347	-58.342	-49.557	5.157
2200	14.136	33.272	22.474	23.754	-58.522	-49.133	4.881
2300	14.272	33.903	22.958	25.174	-58.707	-48.705	4.628
2400	14.406	34.513	23.427	26.608	-58.898	-48.266	4.395
2495	14.534	35.075	23.859	27.983	-59.084	-47.837	4.190
2495	14.534	35.075	23.859	27.983	-64.323	-47.837	4.190
2500	14.541	35.104	23.882	28.056	-64.320	-47.805	4.179
2600	14.674	35.677	24.325	29.516	-64.259	-47.148	3.963
2700	14.808	36.233	24.755	30.990	-64.185	-46.490	3.763
2800	14.941	36.774	25.175	32.478	-64.098	-45.836	3.577
2900	15.073	37.301	25.584	33.979	-64.001	-45.186	3.405
3000	15.206	37.814	25.983	35.492	-63.893	-44.539	3.245
3100	15.338	38.315	26.373	37.020	-63.[illegible]71	-43.896	3.095
3200	15.470	38.804	26.754	38.560	-63.[illegible]	-43.256	2.954
3300	15.602	39.282	27.126	40.114	-63.4[illegible]	-42.622	2.823
3400	15.733	39.750	27.491	41.680	-63.3[illegible]	-41.992	2.699
3500	15.865	40.206	27.848	43.260	-63.173	-41.367	2.583
3600	15.996	40.656	28.197	44.853	-62.994	-40.744	2.473
3700	16.128	41.097	28.540	46.460	-62.803	-40.130	2.370
3800	16.259	41.528	28.876	48.079	-62.601	-39.519	2.273
3900	16.390	41.952	29.206	49.711	-62.388	-38.916	2.181

15 June 1963 HLS

HAFNIUM CARBIDE (HfC) (CONDENSED PHASE) gfw = 190.511

$\Delta H^\circ_{f298.15}$ = -55.0 kcal gfw^{-1} $S^\circ_{298.15}$ = 9.852 cal deg K^{-1} gfw^{-1}

T_m = 3900°K

$H^\circ_{298.15}-H^\circ_0$ = 1.494 kcal gfw^{-1}

$C^\circ_p = 11.3404 + 1.30\times10^{-3}\,T - 3.112\times10^{5}\,T^{-2}$ cal deg K^{-1} gfw^{-1}

298.15°K $\leq T \leq$ 3900°K

Structure

Face-centered-cubic NaCl-type.

Heat of Formation

Intermediate value is based on equilibrium data from Zhelankin et al,[1] vaporization data of Coffman et al,[2] and calorimetry value of Kelley.[3]

Heat Capacity and Entropy

Low-temperature data are estimated.[4] High-temperature data have been evaluated by Shomate method using data from Coffman et al[2] and Neel et al.[5] Data are extrapolated to 3900°K.

Melting and Vaporization

Melting point is estimated from observations of Bowman[6] and data of Avarbe et al.[7]

References

1. Zhelankin, V. I. et al, Russ. J. Phys. Chem. 33, 251-253 (1959).
2. Coffman, J. A. et al, WADD TR 60-646, Part II (January 1963).
3. Kelley, K. K., private communication.
4. Schick, H. L., et al, Vol. 1, this work, section IVB9.2b1; also see section IIID.
5. Neel, D. S., et al, WADD TR 60-924 (1961).
6. Bowman, M., discussions at A. D. Little colloquium (28-29 January 1963).
7. Avarbe, P. G., et al, Zh. Prik. Khim. 35, 1976 (1962).

HAFNIUM CARBIDE (HFC) (CONDENSED PHASE) GFW = 190.511

SUMMARY OF UNCERTAINTY ESTIMATES

T °K	C_p (cal/°K gfw)	S_T	$-(G_T - H_{298})/T$	$H_T - H_{298}$ (kcal/gfw)	ΔH_f	ΔG_f	Log K_f
298.15	± 0.500	± 0.500	± 0.500	± 0.000	±5.000		
1000	± 0.500	± 1.105	± 0.754	± 0.351			
1000	± 1.000	± 1.105	± 0.754	± 0.351			
2000	± 1.000	± 1.798	± 1.123	± 1.351			
2000	± 2.000	± 1.798	± 1.123	± 1.351			
3000	± 2.000	± 2.609	± 1.492	± 3.351			
3900	± 2.000	± 3.134	± 1.813	± 5.151			

DIMOLYBDENUM CARBIDE — CONDENSED PHASE — CMo_2

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Mo from 0° to 2890°K, Liquid Mo from 2890° to 4965°K, Gaseous Mo from 4965° to 6000°K, Solid C; Solid Mo_2C from 0° to 2693°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (kcal gfw)	ΔH_f° (kcal gfw)	ΔF_f° (kcal gfw)	Log K_p
0							
298.15	12.553	17.100	17.100	0.000	-11.535	-12.155	8.910
300	12.610	17.178	17.100	0.023	-11.538	-12.159	8.858
400	14.710	21.131	17.625	1.402	-11.573	-12.359	6.753
500	15.834	24.544	18.676	2.934	-11.576	-12.551	5.486
600	16.573	27.500	19.906	4.557	-11.575	-12.751	4.644
700	17.131	30.099	21.180	6.243	-11.584	-12.946	4.042
800	17.592	32.417	22.443	7.980	-11.586	-13.141	3.590
900	17.996	34.513	23.669	9.759	-11.594	-13.334	3.238
1000	18.366	36.428	24.851	11.578	-11.601	-13.528	2.956
1100	18.713	38.195	25.984	13.432	-11.630	-13.720	2.726
1200	19.044	39.838	27.071	15.320	-11.678	-13.906	2.533
1300	19.365	41.375	28.113	17.240	-11.747	-14.091	2.369
1400	19.677	42.821	29.112	19.192	-11.831	-14.268	2.227
1500	19.984	44.189	30.072	21.176	-11.911	-14.439	2.104
1600	20.286	45.489	30.996	23.189	-12.028	-14.602	1.994
1700	20.585	46.728	31.885	25.233	-12.172	-14.762	1.898
1800	20.881	47.913	32.743	27.306	-12.346	-14.908	1.810
1900	21.174	49.049	33.571	29.409	-12.553	-15.044	1.730
2000	21.466	50.143	34.373	31.541	-12.796	-15.173	1.658
2100	21.757	51.197	35.149	33.702	-13.078	-15.283	1.590
2200	22.047	52.216	35.902	35.892	-13.405	-15.381	1.528
2300	22.335	53.203	36.632	38.111	-13.776	-15.461	1.469
2400	22.623	54.159	37.343	40.359	-14.197	-15.526	1.414
2500	22.910	55.089	38.034	42.636	-14.672	-15.568	1.361
2600	23.197	55.993	38.708	44.941	-15.206	-15.599	1.311
2693	23.463	56.813	39.319	47.111	-15.754	-15.604	1.266

15 September 1963 — DFA

DIMOLYBDENUM CARBIDE (Mo_2C) (CONDENSED PHASE) gfw = 203.91

$\Delta H^\circ_{f298.15}$ = -11.54 kcal gfw^{-1} $S^\circ_{298.15}$ = 17.10 cal deg K^{-1}gfw^{-1}

T_m = 2693°K

$C^\circ_p = 15.92 + (2.82 \times 10^{-3})\ T - (3.74 \times 10^5) T^{-2}$ cal deg K^{-1} gfw^{-1}

$298.15°K \leq T \leq 2693°K$

Structure

Dimolybdenum carbide has a hexagonal close-packed structure with a = 3.002 A and c = 4.724 A [1].

Heat of Formation

The heat of formation was calculated from the free-energy functions and the free energy of formation at 1270°K that was determined by Gleiser and Chipman.[2]

Heat Capacity and Entropy

The heat capacity and entropy are estimates of Krikorian.[3]

Melting and Vaporization

The melting temperature was determined by Nadler and Kempter.[4]

References

1. Hansen, M., Constitution of Binary Alloys, McGraw-Hill, New York (1958).
2. Gleiser, M. and J. Chipman, J. Phys. Chem. 66, 1539 (1962).
3. Krikorian, O., Estimation of High Temperature Heat Capacities of Carbides, UCRL-6785 (1962).
4. Nadler, M.R. and C.P. Kempter, J. Phys. Chem., 64, 1468 (1960).

NIOBIUM CARBIDE — CONDENSED PHASE — CNb

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Nb from 0° to 2741°K, Liquid Nb from 2741° to 5032°K, Gaseous Nb from 5032° to 6000°K, Solid C, Solid NbC from 0° to 3753°K, Liquid NbC from 3753° to 6000°K.

T °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(G_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.258	-33.342	-33.342	INFINITE
298.15	8.886	8.700	8.700	0.000	-33.600	-33.105	24.266
300	8.919	8.755	8.700	0.016	-33.599	-33.102	24.114
400	10.137	11.509	9.067	0.977	-33.484	-32.953	18.004
500	10.793	13.848	9.796	2.026	-33.363	-32.835	14.351
600	11.228	15.856	10.643	3.128	-33.258	-32.740	11.925
700	11.559	17.613	11.515	4.268	-33.171	-32.660	10.196
800	11.835	19.175	12.377	5.438	-33.098	-32.593	8.904
900	12.078	20.583	13.212	6.634	-33.037	-32.533	7.900
1000	12.301	21.867	14.014	7.853	-32.981	-32.481	7.098
1100	12.511	23.050	14.782	9.094	-32.930	-32.432	6.443
1200	12.712	24.147	15.518	10.355	-32.881	-32.390	5.899
1300	12.907	25.172	16.221	11.636	-32.835	-32.351	5.438
1400	13.097	26.135	16.895	12.936	-32.787	-32.313	5.044
1500	13.283	27.045	17.542	14.255	-32.737	-32.283	4.703
1600	13.468	27.909	18.163	15.593	-32.[illegible]84	-32.254	4.406
1700	13.650	28.731	18.761	16.949	-32.626	-32.230	4.143
1800	13.830	29.516	19.337	18.323	-32.565	-32.209	3.910
1900	14.010	30.268	19.892	19.715	-32.499	-32.188	3.702
2000	14.188	30.992	20.429	21.125	-32.427	-32.174	3.516
2100	14.366	31.688	20.949	22.552	-32.350	-32.164	3.347
2200	14.543	32.361	21.452	23.998	-32.267	-32.157	3.194
2300	14.719	33.011	21.941	25.461	-32.178	-32.156	3.055
2400	14.895	33.641	22.415	26.942	-32.084	-32.155	2.928
2500	15.071	34.253	22.877	28.440	-31.983	-32.160	2.811
2600	15.246	34.847	23.326	29.956	-31.877	-32.170	2.704
2700	15.421	35.426	23.763	1.489	-31.764	-32.182	2.605
2741	15.492	35.659	23.939	32.123	-31.715	-32.188	2.566
2741	15.492	35.659	23.939	32.123	-38.115	-32.188	2.566
2800	15.595	35.990	24.190	33.040	-38.025	-32.063	2.502
2900	15.770	36.540	24.606	34.608	-37.861	-31.851	2.400
3000	15.944	37.078	25.013	36.194	-37.680	-31.650	2.306
3100	16.118	37.603	25.411	37.797	-37.483	-31.452	2.217
3200	16.292	38.118	25.800	39.417	-37.271	-31.261	2.135
3300	16.466	38.622	26.181	41.055	-37.[illegible]	-31.079	2.058
3400	16.640	39.116	26.554	42.711	-36.[illegible]	-30.897	1.986
3500	16.813	39.601	26.920	44.383	-36.[illegible]	-30.730	1.919
3600	16.987	40.077	27.279	46.073	-36.263	-30.569	1.856
3700	17.160	40.545	27.631	47.781	-35.971	-30.414	1.796
3753	17.252	40.789	27.815	48.693	-35.810	-30.335	1.766
3753	17.252	46.651	27.815	70.693	-13.810	-30.335	1.766
3800	17.252	46.866	28.049	71.503	-13.666	-30.541	1.756
3900	17.252	47.314	28.538	73.229	-13.359	-30.995	1.737
4000	17.252	47.751	29.012	74.954	-13.054	-31.444	1.716
4100	17.252	48.177	29.473	76.679	-12.751	-31.911	1.701
4200	17.252	48.593	29.925	78.404	-12.4[illegible]0	-32.382	1.685
4300	17.252	48.999	30.364	80.129	-12.1[illegible]	-32.860	1.670
4400	17.252	49.395	30.792	81.855	-11.852	-33.345	1.656
4500	17.252	49.783	31.210	83.580	-11.556	-33.839	1.643
4600	17.252	50.162	31.618	85.305	-11.262	-34.336	1.631
4700	17.252	50.533	32.016	87.030	-10.969	34.841	1.620
4800	17.252	50.896	32.406	88.755	-10.679	-35.354	1.610
4900	17.252	51.252	32.787	90.481	-10.389	-35.869	1.600
5000	17.252	51.601	33.159	92.206	-10.102	-36.390	1.591
5031.58	17.252	51.709	33.276	92.751	-10.012	-36.624	1.591
5031.58	17.252	51.709	33.276	92.751	-172.[illegible]85	-36.624	1.591
5100	17.252	51.942	33.524	93.931	-172.433	-34.768	1.490
5200	17.252	52.277	33.882	95.656	-172.217	-32.071	1.348
5300	17.252	52.606	34.232	97.381	-172.008	-29.381	1.211
5400	17.252	52.928	34.575	99.107	-171.805	-26.686	1.080
5500	17 252	53.245	34.91	100.832	-171.612	-24.008	0.954
5600	17.252	53.556	35.241	102.557	-171.424	-21.330	0.832
5700	17.252	53.861	35.566	104.282	-171.244	-18.649	0.715
5800	17.252	54.161	35.884	106.007	171.070	-15.968	0.602
5900	17.252	54.456	36.196	107.733	-170.901	-13.298	0.493
6000	17.252	54.746	36.503	109.458	-170.739	-10.632	0.387

15 June 196[illegible] HLS

NIOBIUM CARBIDE (NbC) (CONDENSED PHASE) gfw = 104.921

$\Delta H^{\circ}_{f298.15}$ = -33.6 kcal gfw^{-1}

$S^{\circ}_{298.15}$ = 8.7 cal deg K^{-1} gfw^{-1}

T_m = 3753°K

ΔH_m = 22.000 kcal gfw^{-1}

$H^{\circ}_{298.15} - H^{\circ}_0$ = 1.258 kcal gfw^{-1}

$C^{\circ}_p = 10.79 + 1.726 \times 10^{-3} T - 2.15 \times 10^5 T^{-2}$ cal deg K^{-1} gfw^{-1}

298.15°K $\le$ T $\le$ 1840°K

Structure

Cubic NaCl B1-type with a variable range of homogeneity.

Heat of Formation

Combustion data reported by Huber et al[1] have been used.

Heat Capacity and Entropy

Low-temperature data are estimated. High-temperature data of Gel'd and Kusenko are extrapolated to the melting point.[2] Heat capacity of liquid is estimated equal to the heat capacity of solid at the melting point.

Melting and Vaporization

Heat of fusion is estimated.

References

1. Huber, E. J., Jr., et al, J. Phys. Chem. 65, 1846 (1961).

2. Gel'd, P. V. and F. G. Kusenko, Izv. A. N. SSSR O.T.N. Met. i Top. (2), 79-86 (1960).

NIOBIUM CARBIDE (NbC) (CONDENSED PHASE) gfw = 104.921

SUMMARY OF UNCERTAINTY ESTIMATES

T °K	C_p (cal °K gfw)	S_T (cal °K gfw)	$-(G_T - H_{298})/T$ (cal °K gfw)	$H_T - H_{298}$ (Kcal gfw)	ΔH_f (Kcal gfw)	ΔG_f (Kcal gfw)	Log K_p
298.15	± 0.500	± 0.500	± 0.500	± 0.000	± 0.800		
1000	± 0.500	± 1.105	± 0.754	± 0.351			
1000	± 1.000	± 1.105	± 0.754	± 0.351			
2000	± 1.000	± 1.798	± 1.123	± 1.351			
3000	± 1.000	± 2.204	± 1.420	± 2.351			
3753	± 1.000	± 2.428	± 1.601	± 3.104			
3753	± 2.000	± 3.760	± 1.601	± 8.104			
4000	± 2.000	± 3.867	± 1.738	± 8.598			
5000	± 2.000	± 4.334	± 2.214	± 10.598			
6000	± 2.000	± 4.698	± 2.599	± 12.598			

DINIOBIUM CARBIDE — CONDENSED PHASE — CNb_2

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Nb from 0° to 2741°K, Liquid Nb from 2741° to 5032°K, Gaseous Nb from 5032° to 6000°K, Solid C, Solid Nb_2C from 0° to 3363°K.

	cal/°K gfw			Kcal/gfw			
T °K	C_p	S_T	$-(G_T - H_{298})/T$	$H_T - H_{298}$	ΔH_f	ΔF_f	Log K_p
0	0.000	0.000	INFINITE	-2.472	-46.292	-46.292	INFINITE
298.15	14.468	16.000	16.000	0.000	-46.600	-45.599	33.423
300	14.502	16.090	16.000	0.027	-46.599	-45.592	33.212
400	15.799	20.460	16.587	1.549	-46.523	-45.267	24.731
500	16.560	24.073	17.734	3.169	-46.440	-44.964	19.653
600	17.111	27.143	19.057	4.854	-46.371	-44.675	16.272
700	17.562	29.815	20.403	6.588	-46.318	-44.397	13.861
800	17.960	32.166	21.731	8.365	-46.276	-44.126	12.054
900	18.327	34.323	23.013	10.179	-46.245	-43.859	10.650
1000	18.675	36.272	24.243	12.029	-46.215	-43.597	9.528
1100	19.011	38.068	25.419	13.914	-46.187	-43.334	8.609
1200	19.338	39.736	26.543	15.831	-46.158	-43.077	7.845
1300	19.659	41.297	27.619	17.781	-46.129	-42.822	7.199
1400	19.975	42.765	28.649	19.763	-46.095	-42.567	6.645
1500	20.289	44.154	29.637	21.776	-46.056	-42.317	6.165
1600	20.600	45.473	30.586	23.821	-46.011	-42.070	5.746
1700	20.909	46.732	31.499	25.896	-45.958	-41.826	5.377
1800	21.217	47.935	32.379	28.002	-45.899	-41.585	5.049
1900	21.523	49.091	33.228	30.139	-45.832	-41.345	4.755
2000	21.829	50.203	34.049	32.307	-45.755	-41.110	4.492
2100	22.134	51.275	34.844	34.505	-45.670	-40.880	4.254
2200	22.438	52.312	35.615	36.734	-45.576	-40.658	4.039
2300	22.741	53.316	36.362	38.993	-45.473	-40.434	3.842
2400	23.044	54.290	37.089	41.282	-45.363	-40.218	3.662
2500	23.347	55.237	37.796	43.601	-45.242	-40.002	3.497
2600	23.650	56.158	38.485	45.951	-45.113	-39.798	3.345
2700	23.952	57.057	39.156	[illegible]8.331	-44.973	-39.596	3.205
2741	24.076	57.419	39.427	49.316	-44.912	-39.517	3.151
2741	24.076	57.419	39.427	49.316	-57.712	-39.517	3.151
2800	24.254	57.933	39.811	50.742	-57.585	-39.124	3.054
2900	24.556	58.790	40.451	53.182	-57.349	-38.468	2.899
3000	24.857	59.627	41.076	55.653	-57.083	-37.825	2.755
3100	25.159	60.447	41.688	58.154	-56.788	-37.185	2.621
3200	25.460	61.251	42.287	60.685	-56.435	-36.562	2.497
3300	25.761	62.039	42.873	[illegible].246	-56.[illegible]	-35.944	2.380
3363	25.951	62.526	43.237	64.875	-55.8[illegible]	-35.563	2.311

15 June 1963 HLS

DINIOBIUM CARBIDE (Nb_2C) (CONDENSED PHASE) gfw = 197.831

$\Delta H^\circ_{f298.15} = -46.6$ kcal gfw^{-1} $S^\circ_{298.15} = 16.0$ cal deg K^{-1} gfw^{-1}

$T_m = T$ (peritectic) = 3363°K

$H^\circ_{298.15} - H^\circ_0 = 2.472$ kcal gfw^{-1}

$C^\circ_p = 15.88 + 3.0 \times 10^{-3} T - 2.050 \times 10^{5} T^{-2}$ cal deg K^{-1} gfw^{-1}

$298.15°K \leq T \leq 1890°K$

Structure

Hexagonal close-packed type with a variable range of homogeneity.

Heat of Formation

Huber et al[1] have used bomb calorimetry to obtain the heat of formation.

Heat Capacity and Entropy

Entropy at 298.15°K has been estimated. High-temperature heat-capacity data of Gel'd and Kusenko[2] have been extrapolated to peritectic temperature.

References

1. Huber, E. J., Jr., et al, J. Phys. Chem. 65, 1846 (1961).

2. Gel'd, P. V. and F. G. Kusenko, Izv. Akad. Nauk SSSR OTN Met. i Top. 1960, 79-86 (1960).

DINIOBIUM CARBIDE (Nb_2C) (CONDENSED PHASE) GFW = 197.831

SUMMARY OF UNCERTAINTY ESTIMATES

T °K	C_p (cal/°K gfw)	S_T	$-(F_T - H_{298})/T$	$H_T - H_{298}$ (Kcal/gfw)	ΔH_f	ΔF_f	Log K_p
298.15	± 0.500	± 1.500	± 1.500	± 0.000	± 2.000		
1000	± 0.500	± 2.105	± 1.754	± 0.351			
1000	± 1.000	± 2.105	± 1.754	± 0.351			
2000	± 1.000	± 2.798	± 2.123	± 1.351			
2000	± 1.000	± 2.798	± 2.123	± 1.351			
3000	± 1.000	± 3.204	± 2.420	± 2.351			
3363	± 1.000	± 3.318	± 2.511	± 2.744			

TABLE 113

SILICON CARBIDE CONDENSED PHASE **CSi**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Si from 0 to 1690 °K, Liquid Si from 1690° to 3566 °K, Gaseous Si from 3566° to 6000 °K, Solid C, Solid SiC from 0° to 3103 °K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-0.781	-16.260	-16.260	INFINITE
298.15	6.418	3.970	3.970	0.000	-16.500	-15.928	11.675
300	6.472	4.010	3.970	0.012	-16.501	-15.924	11.600
400	8.423	6.175	4.252	0.769	-16.498	-15.731	8.594
500	9.424	8.173	4.840	1.666	-16.469	-15.542	6.793
600	10.051	9.950	5.547	2.642	-16.445	-15.360	5.595
700	10.501	11.535	6.291	3.671	-16.432	-15.180	4.739
800	10.857	12.961	7.037	4.739	-16.428	-15.002	4.098
900	11.159	14.257	[illegible]	5.840	-16.431	-14.823	3.599
1000	11.426	15.447	8.478	6.970	-16.436	-14.645	3.201
1100	11.671	16.548	9.162	8.125	-16.443	-14.465	2.874
1200	11.901	17.573	9.821	9.303	-16.450	-14.286	2.602
1300	12.121	18.535	10.454	10.505	-16.455	-14.104	2.371
1400	12.332	19.441	11.064	11.727	-16.456	-13.923	2.173
1500	12.538	20.299	[illegible]	12.971	-16.453	-13.741	2.002
1600	12.740	21.114	12.218	14.235	-16.444	-13.562	1.852
1690	12.916	21.816	12.710	15.389	[illegible]	-13.399	1.733
1690	12.918	21.816	12.710	15.389	-28.380	-13.399	1.733
1700	12.938	21.893	12.764	15.519	-28.377	-13.311	1.711
1800	13.134	22.638	13.292	16.822	-28.356	-12.425	1.509
1900	13.327	[illegible]	13.803	18.145	-28.326	-11.541	1.327
2000	13.519	24.041	14.298	19.488	-28.285	-10.660	1.165
2100	13.709	24.706	14.777	20.849	-28.226	-9.778	1.018
2200	13.899	25.348	15.243	22.230	-28.152	-8.901	0.884
2300	14.087	25.970	15.696	23.629	-28.060	-8.031	0.763
2400	14.275	26.573	16.137	25.047	-27.953	-7.162	0.652
2500	14.462	27.160	16.565	26.484	-27.827	-6.298	0.551
2600	14.648	27.731	16.985	[illegible]	-27.687	-5.440	0.457
2700	14.834	28.287	17.393	29.413	-27.528	-4.588	0.371
2800	15.020	28.830	17.792	30.906	-27.352	-3.740	0.292
2900	15.205	29.360	18.182	32.417	-27.160	-2.902	0.219
3000	15.390	29.879	18.563	33.947	-26.951	-2.067	0.151
3100	15.574	30.386	18.936	35.495	-26.724	-1.242	0.088
3103	15.580	30.401	18.947	35.542	-26.716	-1.215	0.086

31 December 1963 HLS

SILICON CARBIDE (β-SiC) (CONDENSED PHASE) gfw = 40.101

$\Delta H^o_{f,\,298.15}$ = -16.5 kcal gfw^{-1} $S^o_{298.15}$ = 3.97 cal degK^{-1}gfw^{-1}

$T_{peritectic}$ = 3103°K

$H^o_{298.15} - H^o_0$ = 0.781 kcal gfw^{-1}

$C^o_p = 9.97 + 1.82 \times 10^{-3}T - 3.64 \times 10^5 T^{-2}$ cal degK^{-1}gfw^{-1} 298.15°K $\leq$ T $\leq$ 3103°K

Structure

β-SiC has a cubic structure. The temperature of transformation to the high temperature, i. e., hexagonal or α-form of SiC, is ill defined. Present table gives data for only cubic-SiC, but data for hexagonal SiC are probably not very different.

Heat of Formation

A variety of calorimetric, Si-C-O equilibria, vaporization, solubility, and phase-diagram data reviewed. Final choice based on Si-C-O equilibria.[1,2,3] See volume 1, this report (section IVB25.2) for details.

Heat Capacity and Entropy

Low-temperature data from Kelley and King.[4] High-temperature data from Kelley.[5]

Melting and Vaporization

Peritectic decomposition value from Scace and Slack.[6]

References

1. Baird, J. D. and J. Taylor, Trans. Faraday Soc. 54, 526 (1958).
2. Kay, D. and J. Taylor, Trans Faraday Soc. 56, 1372 (1960).
3. Rein, R. and J. Chipman, J. Phys. Chem. 67, 839 (1963).
4. Kelley, K. and E. King, U. S. Bur. Mines, Bull. 592 (1961).
5. Kelley, K., U. S. Bur. Mines, Bull. 584 (1960).
6. Scace, R. and G. Slack, J. Chem. Phys. 30, 1551 (1959).

SILICON CARBIDE (SiC) (CONDENSED PHASE) GFW = 40.101

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw			kcal/gfw			
	C^o_p	S_T	$-(F_T - H_{298})/T$	$H_T - H_{298}$	ΔH_f	ΔF_f	Log K_p
298.15	± 0.100	± 0.020	± 0.020	± 0.000	± 2.000		
1000	± 0.100	± 0.141	± 0.071	± 0.070			
1000	± 0.500	± 0.141	± 0.071	± 0.070			
2000	± 0.500	± 0.488	± 0.202	± 0.570			
2000	± 2.000	± 0.488	± 0.202	± 0.570			
3000	± 2.000	± 1.299	± 0.442	± 2.570			
3103	± 2.000	± 1.366	± 0.471	± 2.776			

TANTALUM CARBIDE CONDENSED PHASE **CTa**

Reference State for Calculating ΔH_f, ΔF_f, and Log K_p: Solid Ta from 0° to 3270°K, Liquid Ta from 3270° to 5706°K, Gaseous Ta from 5706° to 6000°K, Solid C, Solid TaC from 0° to 4273°K, Liquid TaC from 4273° to 6000°K

T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
	cal/°K gfw			kcal/gfw			
0	0.000	0.000	INFINITE	-1.557	-34.547	-34.547	INFINITE
298.15	8.790	10.110	10.110	0.000	-34.600	-34.251	25.106
300	8.824	10.164	10.110	0.016	-34.599	-34.249	24.949
400	10.118	12.901	10.475	0.971	-34.509	-34.146	18.655
500	10.862	15.245	11.200	2.022	-34.410	-34.066	14.890
600	11.391	17.274	12.047	3.136	-34.316	-34.007	12.386
700	11.817	19.063	12.924	4.297	-34.229	-33.962	10.603
800	12.189	20.665	13.793	5.498	-34.143	-33.930	9.269
900	12.529	22.121	14.639	6.734	-34.054	-33.908	8.234
1000	12.850	23.458	15.455	8.003	-33.957	-33.898	7.408
1100	13.158	24.697	16.239	9.303	-33.849	-33.896	6.734
1200	13.457	25.855	16.993	10.634	-33.729	-33.906	6.175
1300	13.750	26.943	17.717	11.994	-33.597	-33.927	5.703
1400	14.038	27.973	18.413	13.384	-33.448	-33.956	5.301
1500	14.323	28.951	19.083	14.802	-33.287	-33.998	4.953
1600	14.606	29.885	19.729	16.248	-33.110	-34.051	4.651
1700	14.886	30.779	20.353	17.723	-32.915	-34.115	4.386
1800	15.166	31.637	20.956	19.226	-32.706	-34.191	4.151
1900	15.444	32.465	21.541	20.756	-32.481	-34.283	3.943
2000	15.721	33.264	22.107	22.314	-32.243	-34.384	3.757
2100	15.997	34.038	22.657	23.900	-31.990	-34.497	3.590
2200	16.272	34.788	23.191	25.514	-31.725	-34.620	3.439
2300	16.547	35.518	23.711	27.155	-31.450	-34.759	3.303
2400	16.822	36.228	24.218	28.823	-31.167	-34.910	3.179
2500	17.096	36.920	24.712	30.519	-30.881	-35.070	3.066
2600	17.370	37.596	25.195	[illegible].242	-30.590	-35.245	2.962
2700	17.644	38.257	25.667	33.993	-30.306	-35.429	2.868
2800	17.917	38.903	26.128	35.771	-30.036	-35.625	2.781
2900	18.190	39.537	26.579	37.576	-29.793	-35.827	2.700
3000	18.463	40.158	27.022	39.409	-29.585	-36.043	2.626
3100	18.736	40.768	27.455	41.269	-29.420	-36.259	2.556
3200	19.008	41.367	27.881	43.156	-29.307	-36.482	2.491
3270	19.199	41.780	28.174	44.493	-29.262	-36.637	2.449
3270	19.199	41.780	28.174	44.493	-35.[illegible]	-36.637	2.449
3300	19.281	41.956	28.298	45.071	-35.8[illegible]	-36.646	2.427
3400	19.553	42.536	28.708	47.012	-35.34[illegible]	-36.677	2.357
3500	19.826	43.106	29.112	48.981	-34.836	-36.725	2.293
3600	20.098	43.669	29.508	50.978	-34.303	-36.785	2.233
3700	20.370	44.223	29.898	53.001	-33.746	-36.861	2.177
3800	20.642	44.770	30.283	55.052	-33.162	-36.956	2.125
3900	20.914	45.310	30.661	57.129	-32.554	-37.065	2.077
4000	21.186	45.843	31.034	59.234	-31.919	-37.188	2.032
4100	21.458	46.369	31.402	61.367	-31.258	-37.331	1.990
4200	21.730	46.889	31.764	63.526	-30.573	-37.481	1.956
4273	21.929	47.265	32.026	65.120	-30.0[illegible]	-37.608	1.923
4273	16.000	53.116	32.026	90.120	-5.056	-37.608	1.923
4300	16.000	53.217	32.158	90.552	-5.023	-37.812	1.922
4400	16.000	53.585	32.641	92.152	-4.[illegible]00	-38.578	1.916
4500	16.000	53.944	33.111	93.752	[illegible].779	-39.347	1.911
4600	16.000	54.296	33.567	95.352	-4.660	-40.111	1.906
4700	16.000	54.640	34.012	96.952	-4.542	-40.884	1.901
4800	16.000	54.977	34.445	98.552	-4.427	-41.656	1.897
4900	16.000	55.307	34.868	100.152	-4.313	-42.440	1.893
5000	16.000	55.630	35.280	101.752	-4.201	-43.220	1.889
5100	16.000	55.947	35.682	103.352	-4.092	-43.994	1.885
5200	16.000	56.258	36.075	104.952	-3.984	-44.782	1.882
5300	16.000	56.562	36.458	106.552	-3.878	-45.566	1.879
5400	16.000	56.862	36.833	108.152	-3.774	-46.350	1.876
5500	16.000	57.155	37.200	109.752	-3.673	-47.140	1.873
5600	16.000	57.443	37.559	111.352	-3.573	-47.934	1.871
5700	16.000	57.727	37.911	112.952	-3.476	-48.730	1.868
5706.65	16.000	57.745	37.934	113.058	-3.469	-48.787	1.868
5706.65	16.000	57.745	37.934	113.058	-184.692	-48.787	1.868
5800	16.000	58.005	38.255	114.552	-184.757	-46.560	1.754
5900	16.000	58.278	38.592	116.152	-184.832	-44.182	1.637
6000	16.000	58.547	38.922	117.752	-184.912	-41.794	1.522

15 September 1963 HLS

TANTALUM CARBIDE (TaC) (CONDENSED PHASE) gfw = 192.961

$\Delta H^{\circ}_{f298.15} = -34.6 \pm 0.9$ kcal gfw^{-1} $S^{\circ}_{298.15} = 10.11$ cal degK^{-1} gfw^{-1}

$T_m = 4273$°K $\Delta H_m = 25.$ kcal gfw^{-1}

$H^{\circ}_{298.15} - H^{\circ}_0 = 1.557$ kcal gfw^{-1}

$C^{\circ}_p = 10.347 + 0.0027131T - 2.1033 \times 10^5 T^{-2}$ cal deg K^{-1} gfw^{-1} 298.15°K $\leq T \leq$ 4273°K

$C^{\circ}_p = 16.0$ cal deg K^{-1} gfw^{-1} 4273°K $\leq T \leq$ 6000°K

Structure

TaC exists in a f.c.c. structure with variable homogeneity range.

Heat of Formation

Heat of formation is from Huber *et al.*[1]

Heat Capacity and Entropy

Low-temperature data of Kelley[2] was used. High-temperature data of Neel, *et al*[3] and Mezaki[4] was combined by Shomate method and extrapolated to melting point. Data above melting point was estimated.

Melting and Vaporization

Heat of fusion was estimated.

References

1. Huber, E. J. Jr., *et al*, J. Phys. Chem. 67, 793 (1963).
2. Kelley, K. K., J. Am. Chem. Soc. 62, 818 (1940).
3. Neel, D. S., *et al*, WADD TR 60-924 (1962).
4. Mezaki, R., Thesis, M. S., U. of Wisconsin (1961).

TANTALUM CARBIDE (TaC) (CONDENSED PHASE) GFW = 192.961

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p	S°_T	$-(F^{\circ}_T - H^{\circ}_{298})/T$	$H^{\circ}_T - H^{\circ}_{298}$	ΔH°_f	ΔF°_f	Log K_p
	cal/°K gfw			Kcal/gfw			
298.15	±0.500	±0.080	±0.080	±0.000	±0.900		
1000	±0.500	±0.685	±0.334	±0.351			
1000	±2.000	±0.685	±0.334	±0.351			
2000	±2.000	±2.071	±0.896	±2.351			
3000	±2.000	±2.882	±1.432	±4.351			
4000	±2.000	±3.458	±1.870	±6.351			
4273	±2.000	±3.590	±1.976	±6.897			
4273	±3.000	±4.760	±1.976	±11.897			
5000	±3.000	±5.231	±2.416	±14.078			
6000	±3.000	±5.778	±2.932	±17.078			

DITANTALUM CARBIDE   CONDENSED PHASE CTa_2

Reference State for Calculating ΔH_f, ΔF_f, and Log K_p: Solid Ta from 0° to 3270°K, Liquid Ta from 3270° to 5706°K, Gaseous Ta from 5706° to 6000°K, Solid Ta_2C from 0° to 3773°K

T, °K	$C_p°$	$S_T°$	$-(F°_T - H°_{298})/T$	$H°_T - H°_{298}$	$\Delta H_f°$	$\Delta F_f°$	Log K_p
	cal/°K gfw			Kcal/gfw			
0	0.000	0.000	INFINITE	-2.729	-46.961	-46.961	INFINITE
298.15	14.567	19.500	19.500	0.000	-47.200	-46.693	34.226
300	14.601	19.590	19.500	0.027	-47.199	-46.690	34.012
400	15.931	23.993	20.092	1.561	-47.149	-46.528	25.420
500	16.725	27.639	21.247	3.196	-47.099	-46.378	20.271
600	17.309	30.742	22.577	4.899	-47.058	-46.239	16.842
700	17.793	33.448	23.941	6.655	-47.025	-46.104	14.394
800	18.224	35.852	25.282	8.456	-46.995	-45.975	12.559
900	18.624	38.022	26.579	10.298	-46.960	-45.849	11.133
1000	19.005	40.004	27.824	12.180	-46.916	-45.730	9.994
1100	19.374	41.833	29.016	14.099	-46.858	-45.614	9.062
1200	19.734	43.534	30.155	16.054	-46.789	-45.503	8.287
1300	20.088	45.127	31.246	18.045	-46.705	-45.399	7.632
1400	20.437	46.629	32.292	20.072	-46.604	-45.302	7.072
1500	20.784	48.051	33.296	22.133	-46.493	-45.214	6.587
1600	21.128	49.402	34.260	24.228	-46.366	-45.131	6.164
1700	21.470	50.694	35.189	26.358	-46.222	-45.058	5.792
1800	21.811	51.931	36.085	28.522	-46.067	-44.993	5.463
1900	22.150	53.119	36.951	30.720	-45.897	-44.941	5.169
2000	22.489	54.264	37.788	32.952	-45.720	-44.896	4.906
2100	22.827	55.370	38.599	35.218	-45.533	-44.859	4.668
2200	23.164	56.439	39.386	37.518	-45.340	-44.828	4.453
2300	23.500	57.476	40.150	39.851	-45.147	-44.810	4.258
2400	23.836	58.484	40.893	42.218	-44.955	-44.802	4.080
2500	24.172	59.464	41.616	44.618	-44.779	-44.797	3.916
2600	24.508	60.418	42.321	47.052	-44.610	-44.803	3.766
2700	24.843	61.349	43.009	49.520	-44.476	-44.810	3.627
2800	25.178	62.259	43.680	52.021	-44.390	-44.828	3.499
2900	25.513	63.148	44.336	54.555	-44.376	-44.842	3.379
3000	25.847	64.019	44.978	57.123	-44.453	-44.863	3.268
3100	26.182	64.872	45.606	59.725	-44.635	-44.872	3.163
3200	26.516	65.708	46.221	62.359	-44.941	-44.874	3.065
3270	26.750	66.285	46.644	44.224	[illegible]	-44.865	2.998
3270	26.750	66.285	46.644	64.224	[illegible]	-44.865	2.998
3300	26.850	66.529	46.824	65.028	-58.5	-44.745	2.963
3400	27.184	67.336	47.415	67.729	-58.132	-44.334	2.850
3500	27.518	68.129	47.996	70.465	-57.709	-43.931	2.743
3600	27.852	68.909	48.566	73.233	-57.255	-43.546	2.643
3700	28.186	69.676	49.126	76.035	-56.769	-43.171	2.550
3773	28.430	70.229	49.529	78.102	-56.392	-42.903	2.485

DITANTALUM CARBIDE (Ta_2C) (CONDENSED PHASE) gfw = 373.911

$\Delta H^\circ_{f298.15} = -47.2 \pm 3.4$ kcal gfw^{-1} $S^\circ_{298.15} = 19.5 \pm 1$ cal degK^{-1} gfw^{-1}

$T_m = T_{peritectic} = 3773$ °K

$H^\circ_{298.15} - H^\circ_0 = 2.729$ kcal gfw^{-1}

$C^\circ_p = 15.88 + 3.33 \times 10^{-3}T - 2.050 \times 10^5 T^{-2}$ cal deg K^{-1} gfw^{-1} $298.15\,°K \leq T \leq 3773\,°K$

Structure

Ta_2C is hexagonal with variable range of homogeneity.

Heat of Formation

Combustion value from Huber et al[1]

Heat Capacity and Entropy

Low-temperature and high-temperature data were estimated.

Melting and Vaporization

Peritectic temperature is given by Storms.[2]

References

1. Huber, E. J., Jr., et al, J. Phys. Chem. 67, 793 (1963).
2. Storms, E. K., LAMS-2674, (March 1962).

DITANTALUM CARBIDE (Ta_2C) (CONDENSED PHASE) GFW = 373.911

SUMMARY OF UNCERTAINTY ESTIMATE

T, °K	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]
298.15	±1.000	±1.000	±1.000	±0.000	±3.400		
1000	±1.000	±2.210	±1.508	±0.702			
1000	±3.00	±2.210	±1.506	±0.702			
2000	±3.000	±4.290	±2.432	±3.702			
3000	±3.000	±5.506	±3.272	±6.702			
3773	±3.000	±6.1[illegible]4	±3.803	±9.021			

TABLE 116

THORIUM CARBIDE — CONDENSED PHASE — CTh

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Th from 0° to 2028°K, Liquid Th from 2028° to 5060°K, Gaseous Th from 5060° to 6000°K, Solid C, Solid ThC from 0° to 2898°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	---	---	---	---	---	---	---
298.15	10.198	11.500	11.500	0.000	-7.000	-6.219	4.559
300	10.235	11.563	11.500	0.019	-6.997	-6.214	4.527
400	11.628	14.723	11.922	1.121	-6.808	-5.981	3.268
500	12.373	17.405	12.757	2.324	-6.615	-5.797	2.534
600	12.863	19.707	13.728	3.587	-6.448	-5.649	2.058
700	13.233	21.718	14.729	4.893	-6.310	-5.527	1.726
800	13.538	23.506	15.717	6.231	-6.199	-5.424	1.482
900	13.807	25.116	16.673	7.599	-6.112	-5.332	1.295
1000	14.052	26.584	17.592	8.992	-6.046	-5.250	1.147
1100	14.282	27.934	18.471	10.409	-6.006	-5.172	1.027
1200	14.502	29.186	19.313	11.848	-5.998	-5.098	0.928
1300	14.714	30.355	20.118	13.309	-6.029	-5.021	0.844
1400	14.921	31.453	20.889	14.791	-6.104	-4.941	0.771
1500	15.125	32.490	21.628	16.293	-6.237	-4.855	0.707
1600	15.325	33.472	22.338	17.816	-6. 38	-4.755	0.649
1633	15.391	33.786	22.566	18.322	-6.522	-4.719	0.631
1633	15.391	33.786	22.566	18.322	-7.175	-4.719	0.631
1700	15.523	34.407	23.020	19.358	-7.261	-4.615	0.593
1800	15.719	35.300	23.678	20.920	-7.378	-4.457	0.541
1900	15.914	36.155	24.312	22.502	-7.478	-4.291	0.494
2000	16.108	36.977	24.925	24.103	-7.562	-4.122	0.450
2028	16.162	37.201	25.093	24.555	-7.582	-4.074	0.439
2028	16.162	37.201	25.093	24.555	-11.435	-4.074	0.439
2100	16.301	37.767	25.518	25.724	-11.481	-3.810	0.397
2200	16.493	38.530	26.092	27.363	-11.533	-3.443	0.342
2300	16.684	39.267	26.649	29.022	-11.566	-3.076	0.292
2400	16.875	39.981	27.190	[illegible].700	-11.583	-2.706	0.246
2500	17.065	40.674	27.715	32.397	-11.582	-2.335	0.204
2600	17.255	41.347	28.227	34.113	-11.565	-1.966	0.165
2700	17.445	42.002	28.725	35.848	-11.530	-1.600	0.130
2800	17.634	42.640	29.210	37.602	-11.477	-1.229	0.096
2898	17.820	43.250	29.675	39.339	-11.410	-0.874	0.066

15 September 1963 — MBP

THORIUM CARBIDE (ThC) (CONDENSED PHASE) gfw = 244.061

$\Delta H f^{\circ}_{298.15} = -7 \pm 6$ kcal gfw^{-1} $S^{\circ}_{298.15} = 11.5 \pm 5$ cal deg^{-1} gfw^{-1}

$T_m = 2898 \pm 25$ °K

$C_p^{\circ} = (12.43 \pm .30) + (1.87 \pm .04) \times 10^{-3}T - (2.48 \pm 0.40) \times 10^{5}T^{-2}$ cal degK^{-1} gfw^{-1}
$298\,°K \leq T \leq 2898\,°K$

Face-centered cubic (NaCl type)

Heat of Formation

Measured by Huber and Holley.[1]

Heat Capacity and Entropy

Empirical equation developed by Krikorian.[2]

Melting and Vaporization

Melting point - Wilhelm & Chiotti.[3]

References

1. Huber, E. J., Jr., and C. E. Holley Jr., Paper No. 26, IAEA Symposium, Vienna, June 1962.
2. Krikorian, O. H., UCRL 2888
3. Wilhelm, H., and Chiotti, P., Trans. Am. Soc. Met. 42, 1295 (1950).

THORIUM CARBIDE (ThC) (CONDENSED PHASE) GFW = 244.061

SUMMARY OF UNCERTAINTY ESTIMATES

T °K	C_p	S	$-(G-H_{298})/T$	$H_T - H_{298}$	ΔHf	ΔGf	Log Kp
298.15	±0.256	±0.500	±0.500	±0.000	±6.000		
500	±0.300	±0.645	±0.531	±0.057			
1000	±0.335	±0.865	±0.648	±0.217			
1500	±0.358	±1.006	±0.745	±0.390			
2000	±0.379	±1.112	±0.824	±0.575			
2500	±0.399	±1.198	±0.891	±0.769			
2898	±0.415	±1.258	±0.937	±0.931			

TABLE 117

TITANIUM CARBIDE — CONDENSED PHASE — CTi

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ti from 0° to 1950°K, Liquid Ti from 1950 to 3550°K, Gaseous Ti from 3550° to 6000°K, Solid C, Solid TiC from 0° to 3212°K, Liquid TiC from 3213° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.161	-43.829	-43.829	INFINITE
298.15	8.041	5.790	5.790	0.000	-44.130	-43.266	31.713
300	8.092	5.840	5.790	0.015	-44.130	-43.260	31.514
400	9.912	8.453	6.134	0.928	-44.083	-42.976	23.480
500	10.798	10.770	6.835	1.968	-44.011	-42.707	18.666
600	11.316	12.788	7.663	3.075	-43.955	-42.452	15.463
700	11.659	14.560	8.524	4.225	-43.924	-42.204	13.176
800	11.911	16.134	9.379	5.404	-43.914	-41.960	11.462
900	12.108	17.549	10.209	6.605	-43.925	-41.714	10.129
1000	12.272	18.833	11.008	7.825	-43.951	-41.468	9.062
1100	12.414	20.009	11.774	9.059	-43.994	-41.218	8.189
1155	12.486	20.617	12.181	9.744	-44.022	-41.078	7.773
1155	12.486	20.617	12.181	9.744	-44.972	-41.078	7.773
1200	12.541	21.095	12.506	10.307	-44.998	-40.926	7.453
1300	12.658	22.104	13.206	11.567	-45.065	-40.585	6.823
1400	12.767	23.046	13.876	12.838	-45.140	- 0.237	6.281
1500	12.871	23.930	14.517	14.120	-45.222	-39.885	5.811
1600	12.970	24.764	15.131	15.412	-45.311	-39.525	5.399
1700	13.066	25.553	15.721	16.714	-45.4[illegible]	-39.159	5.034
1800	13.160	26.303	16.289	18.025	-45.5[illegible]	-38.791	4.710
1900	13.251	27.017	16.835	19.346	-45.60[illegible]	-38.415	4.418
1950	13.296	27.362	17.100	20.010	-45.657	-38.223	4.284
1950	13.296	27.362	17.100	20.010	-49.357	-38.223	4.284
2000	13.340	27.699	17.361	20.676	-49.385	-37.940	4.146
2100	13.429	28.352	17.869	22.014	-49.434	-37.366	3.889
2200	13.516	28.976	18.359	23.361	-49.478	-36.791	3.655
2300	13.602	29.581	18.835	24.717	-49.514	-36.216	3.441
2400	13.688	30.162	19.294	26.082	-49.544	-35.632	3.245
2500	13.773	30.722	19.740	27.455	-49.567	-35.052	3.064
2600	13.857	31.264	20.173	28.836	-49.585	-34.471	2.897
2700	13.941	31.785	20.594	30.226	-49.595	-33.892	2.743
2800	14.024	32.277	21.003	31.624	-49.598	-33.308	2.600
2900	14.107	32.761	21.401	33.031	-49.595	-32.727	2.466
3000	14.190	33.[illegible]	21.787	34.446	-49.585	-32.148	2.342
3100	14.273	33.737	22.166	35.869	-49.568	-31.566	2.225
3200	14.355	34.1[illegible]	22.545	37.[illegible]	-49.545	-30.984	2.116
3213	14.366	34.250	22.582	37.487	-49.541	-30.909	2.102
3213	16.000	40.474	22.58[illegible]	57.487	-29.[illegible]	-30.909	2.102
3300	16.000	40.902	23.160	58.879	-29.37	-30.950	2.050
3400	16.000	41.380	23.5[illegible]	60.479	-29.18	-30.999	1.993
3500	16.000	41.843	24.10[illegible]	6[illegible].079	-29.000	-31.057	1.939
3550	16.000	42.070	24.358	62.879	-28.907	-31.087	1.914
3550	16.000	42.070	24.35[illegible]	62.879	-131.3[illegible]	-31.087	1.914
3600	16.000	42.[illegible]	[illegible]	63.679	-131.276	-29.676	1.801
3700	16.000	42.733	[illegible]	65.279	-131.1[illegible]	-26.855	1.586
3800	16.000	43.159	[illegible]	66.879	-130.963	-24.036	1.382
3900	16.000	43.57[illegible]	[illegible]	68.479	-130.890	-21.229	1.190
4000	16.000	43.980	26.4[illegible]	70.079	-130.710	-18.418	1.006
4100	16.000	44.375	26.8[illegible]	[illegible]1.679	-130.60[illegible]	-15.610	0.832
4200	16.000	44.761	27.313	73.279	-130.514	-12.806	0.666
4300	16.000	45.137	27.72[illegible]	74.879	-130.43[illegible]	-10.005	0.508
4400	16.000	45.505	28.17[illegible]	76.479	[illegible]	-7.205	0.358
4500	16.000	45.864	[illegible]	78.07[illegible]	[illegible]	-4.413	0.214
4600	16.000	46.216	28.895	79.679	-130.280	-[illegible].612	0.077
4700	16.000	46.560	29.267	[illegible]	-130.25[illegible]	[illegible].183	-0.055
4800	16.000	46.897	29.631	[illegible].879	-130.236	3.980	-0.181
4900	16.000	47.227	29.986	84.479	-130.230	6.781	-0.302
5000	16.000	47.550	30.334	86.079	-130.234	9.575	-0.419
5100	16.000	47.867	30.67[illegible]	87.679	-130.250	12.37[illegible]	-0.530
5200	16.000	48.178	31.00[illegible]	89.279	-130.274	15.166	-0.637
5300	16.000	48.483	31.336	90.879	-130.307	17.965	-0.741
5400	16.000	48.782	31.65[illegible]	[illegible].479	-130.34[illegible]	20.762	-0.840
5500	16.000	49.07[illegible]	31.97[illegible]	94.079	-130.400	23.564	-0.936
5600	16.000	49.363	[illegible]	95.679	-130.458	26.3[illegible]	-1.029
5700	16.000	49.647	[illegible]	[illegible]	-130.524	29.166	-1.118
5800	16.000	49.925	32.977	98.879	-130.597	31.966	-1.204
5900	16.000	50.1[illegible]	[illegible]	100.479	-130.676	34.771	-1.288
6000	16.000	50.467	[illegible]	102.079	-130.761	37.572	-1.368

31 December 1963 — HLS

TITANIUM CARBIDE (TiC) *(CONDENSED PHASE)* $gfw = 59.911$

$\Delta H^o_{f298.15} = -44.13$ kcal gfw^{-1}

$S^o_{298.15} = 5.79$ cal $degK^{-1} gfw^{-1}$

$T_m = 3213^oK$

$\Delta H_m = 20.0$ kcal gfw^{-1}

$H^o_{298.15} - H^o_0 = 1.101$ kcal gfw^{-1}

$C^o_p = 11.83 + 0.80 \times 10^{-3}T - 3.58 \times 10^5 T^{-2}$ cal $degK^{-1} gfw^{-1}$ $298.15^oK \leq T \leq 3213^oK$

Structure

TiC has an f. c. c. structure (NaCl type) with variable homogeneity range.

Heat of Formation

Several possible values examined in the text. The calorimetric value from Humphrey[1] accepted.

Heat Capacity and Entropy

Low-temperature data from Kelley.[2] High-temperature data by Naylor.[3]

Melting and Vaporization

Heat of fusion estimated.

References

1. Humphrey, G., J. Am. Chem. Soc. 73, 2261 (1951).
2. Kelley, K. K., Ind. Eng. Chem. 36, 865 (1944).
3. Naylor, B., J. Am. Chem. Soc. 68, 370 (1946).

TUNGSTEN CARBIDE CONDENSED PHASE **CW**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p. Solid W from 0° to 3650°K, Liquid W from 3650° to 5891°K, Gaseous W from 5891° to 6000°K, Solid C, Solid WC from 0° to 3058°K.

T °K	cal/°K gfw			kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0							
298.15	9.869	9.500	9.500	0.000	-8.400	-8.493	6.225
300	9.910	9.561	9.500	0.018	-8.397	-8.493	6.187
400	11.419	12.646	9.910	1.094	-8.155	-8.551	4.672
500	12.228	15.288	10.729	2.280	-7.889	-8.691	3.799
600	12.762	17.567	11.683	3.551	-7.623	-8.865	3.229
700	13.165	19.566	12.669	4.828	-7.365	-9.105	2.843
800	13.499	21.346	13.645	6.161	-7.113	-9.358	2.556
900	13.793	22.954	14.591	7.526	-6.863	-9.670	2.348
1000	14.062	24.421	15.502	8.919	-6.608	-9.976	2.180
1100	14.315	25.773	16.375	10.338	-6.352	-10.347	2.056
1200	14.556	27.029	17.211	11.782	-6.090	-10.697	1.948
1300	14.789	28.204	18.012	13.249	-5.831	-11.118	1.869
1400	15.017	29.308	18.780	14.739	-5.570	-11.536	1.801
1500	15.241	30.352	19.517	16.252	-5.308	-11.971	1.744
1600	15.461	31.342	20.225	17.788	-5.045	-12.424	1.697
1700	15.679	32.286	20.907	19.345	-4.779	-12.893	1.657
1800	15.895	33.169	21.564	20.923	-4.[illegible]13	-13.377	1.624
1900	16.110	34.054	22.199	22.524	-4.241	-13.878	1.596
2000	16.323	34.885	22.813	24.145	-3.968	-14.394	1.573
2100	16.535	35.687	23.407	25.788	-3.689	-14.918	1.553
2200	16.747	36.461	23.983	27.452	-3.409	-15.462	1.536
2300	16.957	37.210	24.542	29.137	-3.123	-16.018	1.522
2400	17.167	37.936	25.065	30.844	-2.834	-16.584	1.510
2500	17.377	38.641	25.613	32.571	-2.540	-17.160	1.500
2600	17.586	39.327	26.127	34.319	-2.244	-17.752	1.492
2700	17.795	39.995	26.629	36.088	-1.942	-18.355	1.486
2800	18.004	40.646	27.116	37.876	-1.636	-18.967	1.480
2900	18.212	41.261	27.595	39.689	-1.326	-19.591	1.476
3000	18.420	41.902	28.062	41.521	-1.012	-20.229	1.474
3058	18.542	42.256	28.328	42.592	-0.828	-20.604	1.472

15 June 1963 DFA

TUNGSTEN CARBIDE (WC) (CONDENSED PHASE) gfw = 195.871

$\Delta H^{\circ}_{f298.15} = -8.4$ kcal gfw^{-1} $S^{\circ}_{298.15} = 9.5$ cal deg K^{-1} gfw^{-1}

$T_m = 3058\,^{\circ}K$

$C^{\circ}_p = 12.27 + 2.06 \times 10^{-3}T - 2.68 \times 10^{5}T^{-2}$ cal deg K^{-1} gfw^{-1} $298.15\,^{\circ}K \leq T \leq 3058\,^{\circ}K$

Structure

The structure of α-WC is simple hexagonal. A high-temperature form with face-centered cubic structure has been reported. See text for details.

Heat of Formation

The heat of formation of -8.4 kcal gfw^{-1} used is that reported by Huff and co-workers[1] who corrected the value reported by McGraw and co-workers.[2]

Heat Capacity and Entropy

No low-temperature heat capacity data have been reported. The value for $S^{\circ}_{298.15}$ is that estimated by Krikorian.[3] The high-temperature heat capacity equation was also estimated by Krikorian.[3]

Melting and Vaporization

Coffman and co-workers[4] investigated the vaporization of WC but were unable to obtain thermodynamic data. The melting point of 3058 °K reported by Sara and Dolloff[5] has been used.

References

1. Huff, G., E. Squitieri, and P. E. Snyder, JACS 70, 3380 (1948).
2. McGraw, L. D., H. Settz, and P. E. Snyder, JACS 69, 329 (1947).
3. Krikorian, O., Estimation of High-Temperature Heat Capacities of Carbides, UCRL 6785 (1962).
4. Coffman, J. A., G. M. Kibler, T. F. Lyon, and B. D. Acchione, WADD-TR-60-646, Part II (1963).
5. Sara, R. V. and R. T. Dolloff, WADD-TR-60-143, Part III (1962).

TUNGSTEN CARBIDE (WC) (CONDENSED PHASE) GFW = 195.871

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw			kcal/gfw			
	C_p	S_T	$-(G_T - H_{298})/T$	$H_T - H_{298}$	ΔH_f	ΔF_f	Log K_p
298.15	± 1.000	± 0.500	± 0.500	± 0.000	± 0.200		
500	± 1.000	± 1.017	± 0.613	± 0.202			
1000	± 1.000	± 1.710	± 1.008	± 0.702			
1500	± 1.000	± 2.116	± 1.314	± 1.202			
2000	± 1.000	± 2.403	± 1.552	± 1.702			
2500	± 1.000	± 2.626	± 1.746	± 2.202			
3000	± 1.000	± 2.809	± 1.908	± 2.702			
3058	± 1.000	± 2.828	± 1.925	± 2.760			

DITUNGSTEN CARBIDE — CONDENSED PHASE — CW_2

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid W from 0° to 3650°K, Liquid W from 3650° to 5891°K, Gaseous W from 5891° to 6000°K, Solid C, Solid W_2C from 0° to 3068°K

T °K	C_p° (cal/°K gfw)	S° (cal/°K gfw)	$-(F^\circ - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ - H^\circ_{298}$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0							
298.15	18.320	19.500	19.500	0.000	-11.000	-11.740	8.605
300	18.373	19.613	19.500	0.034	-10.992	-11.744	8.555
400	20.325	25.201	20.249	1.981	-10.467	-12.054	6.586
500	21.368	29.858	21.719	4.070	-9.899	-12.535	5.479
600	22.053	33.818	23.414	6.243	-9.318	-13.095	4.769
700	22.570	37.258	25.151	8.475	-8.739	-13.795	4.307
800	22.996	40.301	26.858	10.754	-8.163	-14.529	3.969
900	23.370	43.031	28.506	13.073	-7.587	-15.394	3.738
1000	23.712	45.511	30.084	15.427	-7.003	-16.252	3.552
1100	24.032	47.787	31.592	17.814	-6.419	-17.250	3.427
1200	24.338	49.891	33.030	20.233	-5.828	-18.211	3.316
1300	24.634	51.851	34.403	22.682	-5.246	-19.320	3.248
1400	24.922	53.687	35.716	25.160	-4.670	-20.428	3.189
1500	25.205	55.416	36.972	27.666	-4.102	-21.572	3.143
1600	25.484	57.052	38.176	30.200	-3.744	-22.755	3.108
1700	25.760	58.605	39.333	32.763	-2.[illegible]89	-23.974	3.082
1800	26.033	60.085	40.445	35.352	-2.445	-25.224	3.062
1900	26.304	61.500	41.516	37.969	-1.704	-26.504	3.049
2000	26.573	62.856	42.549	40.613	-1.371	-27.814	3.039
2100	26.841	64.159	43.548	43.284	-0.841	-29.144	3.033
2200	27.108	65.414	44.513	45.981	-0.321	-30.507	3.030
2300	27.374	66.625	45.448	48.705	0.197	-31.891	3.030
2400	27.640	67.795	46.355	51.456	0.707	-33.298	3.032
2500	27.904	68.929	47.236	54.233	1.214	-34.722	3.035
2600	28.169	70.028	48.091	57.037	1.713	-36.173	3.040
2700	28.432	71.096	48.924	59.867	2.209	-37.638	3.046
2800	28.696	72.135	49.734	62.723	2.698	-39.120	3.053
2900	28.959	73.147	50.524	65.606	3.183	-40.623	3.061
3000	29.221	74.133	51.299	68.515	3.661	-42.146	3.070
3068	29.400	74.790	51.808	70.508	3.984	-43.186	3.076

15 June 1963 — DFA

DITUNGSTEN CARBIDE (W_2C) (CONDENSED PHASE) gfw = 379.731

$\Delta H^\circ_{f298.15}$ = -11.0 kcal gfw^{-1} $S^\circ_{298.15}$ = 19.5 cal deg K^{-1} gfw^{-1}

T_m = 3068°K

$C_p^\circ = 21.45 + 2.60\times10^{-3}T - 3.48\times10^{5}T^{-2}$ cal deg K^{-1} gfw^{-1} 298.15°K $\leq T \leq$ 3068°K

Structure

The crystal structure of W_2C is simple hexagonal. Lattice parameters are given in the text.

Heat of Formation

The heat of formation of -11.0 kcal gfw^{-1} estimated by Krikorian[1] has been used since no experimental values have been reported.

Heat Capacity and Entropy

No low temperature heat capacity data have been reported. The entropy at 298.15°K is that estimated by Krikorian.[2] The high-temperature heat capacity equation is that estimated by Krikorian.[2]

Melting and Vaporization

No vaporization data have been reported. The melting point of 3068°K reported by Sara and Dolloff[3] has been adopted.

References

1. Krikorian, O., High Temperature Studies, UCRL-2888 (April 1955).
2. Krikorian, O., Estimation of High Temperature Heat Capacities of Carbides, UCRL-6785 (1962).
3. Sara, R. V. and R. T. Dolloff, WADD-TR-60-143, Part III (1962).

DITUNGSTEN CARBIDE (W_2C) (CONDENSED PHASE) GFW = 379.731

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C_p° (cal/deg gfw)	S°_T	$-(G^\circ_T - H^\circ_{298})/T$	$H^\circ_T - H^\circ_{298}$ (kcal/gfw)	ΔH°_f	ΔG°_f	Log K_p
298.15	± 1.400	± 1.000	± 1.000	± 0.000	± 4.000		
500	± 1.400	± 1.724	± 1.159	± 0.283			
1000	± 1.400	± 2.694	± 1.712	± 0.983			
1500	± 1.400	± 3.262	± 2.140	± 1.683			
2000	± 1.400	± 3.665	± 2.473	± 2.383			
2500	± 1.400	± 3.977	± 2.744	± 3.083			
3000	± 1.400	± 4.232	± 2.971	± 3.783			
3068	± 1.400	± 4.264	± 3.000	± 3.878			

ZIRCONIUM CARBIDE — CONDENSED PHASE — CZr

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p Solid Zr from 0° to 2125°K, Liquid Zr from 2125° to 4644°K, Gaseous Zr from 4644° to 6000°K, Solid C. Solid ZrC from 0° to 3693°K, Liquid ZrC from 3693° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.401	-47.836	-47.836	INFINITE
298.15	9.058	7.964	7.964	0.000	-48.000	-47.199	34.596
300	9.098	8.020	7.964	0.017	-47.998	-47.194	34.380
400	10.588	10.868	8.342	1.010	-47.882	-46.943	25.647
500	11.395	13.324	9.099	2.113	-47.771	-46.722	20.421
600	11.935	15.452	9.985	3.281	-47.682	-46.521	16.944
700	12.346	17.324	10.904	4.495	-47.616	-46.333	14.465
800	12.694	18.996	11.811	5.748	-47.564	-46.154	12.608
900	13.000	20.509	12.695	7.033	-47.525	-45.979	11.165
1000	13.282	21.894	13.547	8.347	-47.493	-45.810	10.011
1100	13.548	23.172	14.364	9.687	-47.466	-45.643	9.068
1135	13.672	23.588	14.638	10.167	-47.454	-45.580	8.776
1135	13.672	23.588	14.638	10.167	-48.369	-45.580	8.776
1200	13.803	24.362	15.148	11.056	-48.344	-45.426	8.273
1300	14.051	25.477	15.900	12.449	-48.290	-45.184	7.596
1400	14.293	26.527	16.622	13.866	-48.214	-44.948	7.016
1500	14.530	27.521	17.316	15.308	-48.[illegible]	-44.718	6.515
1600	14.765	28.466	17.984	16.772	-48.027	-44.494	6.077
1700	14.998	29.364	18.627	18.261	-47.902	-44.275	5.692
1800	15.228	30.232	19.248	19.772	-47.760	-44.067	5.350
1900	15.457	31.062	19.848	21.306	-47.598	-43.866	5.045
2000	15.68[illegible]	31.860	20.429	22.863	-47.416	-43.676	4.772
2100	15.912	32.631	20.992	24.443	-47.213	-43.493	4.526
2125	15.968	32.817	21.128	24.884	-47.116	-43.444	4.468
2125	15.968	32.817	21.128	24.884	-52.016	-43.444	4.468
2200	16.137	33.377	21.538	26.045	-51.899	-43.147	4.286
2300	16.363	34.099	22.068	27.670	-51.666	-42.756	4.063
2400	16.587	34.700	22.584	29.318	-51.413	-42.372	3.858
2500	16.812	35.462	23.087	30.988	-51.139	-42.003	3.672
2600	17.036	36.145	23.576	32.680	-50.846	-41.640	3.500
2700	17.259	36.793	24.054	34.395	-50.531	-41.296	3.343
2800	17.482	37.424	24.520	36.132	-50.195	-40.958	3.197
2900	17.705	38.042	24.976	37.892	-49.839	-40.634	3.062
3000	17.928	38.646	25.421	39.673	-49.463	-40.323	2.937
3100	18.151	39.237	25.857	41.477	-49.06[illegible]	-40.024	2.822
3200	18.373	39.817	26.285	43.303	-48.64	-39.741	2.714
3300	18.596	40.386	26.703	45.152	-48.208	-39.469	2.614
3400	18.817	40.944	27.114	47.022	-47.749	-39.211	2.520
3500	19.039	41.493	27.517	48.915	-47.269	-38.967	2.433
3600	19.261	42.032	27.913	50.830	-46.768	-38.737	2.352
3693	19.467	42.526	28.275	52.631	-46.284	-38.539	2.281
3693	19.000	47.942	28.275	72.631	-26.284	-38.539	2.281
3700	19.000	47.978	28.312	72.764	-26.250	-38.558	2.277
3800	19.000	48.484	28.836	74.664	-25.767	-38.899	2.237
3900	19.000	48.978	29.346	76.564	-25.286	-39.248	2.199
4000	19.000	49.459	29.843	78.464	-24.806	-39.612	2.164
4100	19.000	49.926	30.327	80.364	-24.328	-39.989	2.131
4200	19.000	50.386	30.799	82.264	-23.852	-40.377	2.101
4300	19.000	50.833	31.260	84.164	-23.378	-40.776	2.072
4400	19.000	51.270	31.710	86.064	-22.905	-41.189	2.046
4500	19.000	51.697	32.149	87.964	-22.434	-41.605	2.021
4600	19.000	52.114	32.579	88.864	-21.965	-42.038	1.997
4644.05	19.000	52.294	32.764	90.701	-21.758	-42.227	1.987
4644.05	19.000	52.294	32.764	90.701	-157.212	-42.227	1.987
4700	19.000	52.523	32.999	91.764	-157.005	-40.847	1.899
4800	19.000	52.923	33.410	93.664	-156.641	-38.381	1.747
4900	19.000	53.315	33.812	95.564	-156.284	-35.917	1.602
5000	19.000	53.699	34.206	97.464	-155.933	-33.465	1.463
5100	19.000	54.075	34.592	99.364	-155.590	-31.022	1.329
5200	19.000	54.444	34.970	101.264	-155.253	-28.578	1.201
5300	19.000	54.806	35.341	103.164	-154.922	-26.148	1.078
5400	19.000	55.161	35.705	105.064	-154.596	-23.722	0.960
5500	19.000	55.510	36.062	106.964	-154.276	-21.303	0.846
5600	19.000	55.852	36.412	108.864	-153.961	-18.886	0.737
5700	19.000	56.188	36.756	110.764	-153.652	-16.473	0.632
5800	19.000	56.519	37.094	112.664	-153.346	-14.070	0.530
5900	19.000	56.844	37.426	114.564	-153.045	-11.674	0.432
6000	[illegible]	57.163	37.752	116.464	-152.748	-9.276	0.338

15 March 1963 HLS

$\Delta H^o_{f298.15} = -48.0$ Kcal gfw^{-1}

$S^o_{298.15}$ 7.964 cal degK^{-1}gfw^{-1}

$T_m = 3693^oK$

ΔH_m - 20 0 Kcal gfw^{-1}

$H^o_{298.15} - H^o_0 = 1\ 401$ Kcal gfw^{-1}

$C^o_p = 11.336 + 2.207 \times 10^{-3}T - 2\ 610 \times 10^5 T^{-2}$ cal degK^{-1}gfw^{-1}

$298\ 15^oK \leq T \leq \quad 3693^oK$

Structure

ZrC has a cubic, NaCl (B1) type structure.

Heat of Formation

Choice based on vaporization from Knudsen cell by Pollock,[1] and Langmuir vaporization by Pollock[1] and Coffman et al [2]

Heat Capacity and Entropy

Low-temperature data by Westrum[3] and Westrum and Feick [4] High-temperature data based on estimates of Krikorian[5] joined low-temperature data It agreed with available experimental data of Margrave[6] and Southern Res Inst [7]

Melting and Vaporization

Melting temperature from Dolloff and Sara [8] Heat of melting estimated

References

1 Pollock, B D., J Phys Chem 65, 731 (1961)
2. Coffman, J. A. et al, WADD TR-60-646, Pt. II (1961).
3. Westrum, E , in A. D. Little Third Semiannual Prog Rept , Contract AF33(616)-7472 (August 1962)
4 Westrum, E. and G. Feick, Manuscript courtesy of E. Westrum.
5. Krikorian, O H., UCRL-6785 (6 February 1962).
6. Margrave, J , in A. D Little Rept , ASD-TDR-62-204, Pt. I, AD 277500 (April 1962).
7 Neel, D. S. et al, Southern Res Inst , WADD TR-60-924 (February 1962)
8. Dolloff, R. T. and R. V. Sara, Nat. Carbon Co. Prog. Rept. No. 3, Contract AF33(616)-6286 (10 December 1962).

ZIRCONIUM CARBIDE (ZrC) (CONDENSED PHASE) GFW = 103.231

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C_p (cal °K gfw)	S_T	$-(F_T - H_{298})/T$	$H_T - H_{298}$ (Kcal gfw)	ΔH_f	ΔF_f	Log K_p
298.15	± 0.300	± 0.050	± 0.050	± 0.000	± 5.000		
1000	± 0.500	± 0.413	± 0.262	± 0.211			
2000	± 0.850	± 0.898	± 0.443	± 0.911			
3000	± 1.000	± 1.304	± 0.667	± 1.911			
3693	± 1.000	± 1.512	± 0.807	± 2.604			
3693	± 1.000	± 2.865	± 0.807	± 7.604			
4000	± 2.000	± 3.025	± 0.971	± 8.218			
5000	± 2.000	± 3.471	± 1.428	±10.218			
6000	± 2.000	± 3.836	± 1.800	±12.218			

DIATOMIC CARBON — IDEAL MOLECULAR GAS — C_2

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p
Solid Graphite from 0° to 6000°K

T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
	cal/°K gfw			Kcal gfw			
0	0.000	0.000	INFINITE	-2.528	196.636	196.636	INFINITE
298.15	10.312	47.630	47.630	0.000	198.660	185.270	-135.800
300	10.302	47.694	47.630	0.019	198.671	185.186	-134.902
400	9.478	50.548	48.025	1.009	199.169	180.610	-98.676
500	8.878	52.592	48.744	1.924	199.446	175.934	-76.897
600	8.606	54.182	49.523	2.796	199.562	171.218	-62.363
700	8.516	55.501	50.285	3.651	199.567	166.493	-51.979
800	8.512	56.637	51.010	4.502	199.500	161.770	-44.191
900	8.546	57.641	51.692	5.355	199.379	157.062	-38.138
1000	8.599	58.544	52.333	6.212	199.224	152.367	-33.298
1100	8.659	59.366	52.935	7.075	199.041	147.692	-29.342
1200	8.724	60.123	53.503	7.944	198.838	143.032	-26.048
1300	8.791	60.824	54.040	8.819	198.615	138.389	-23.264
1400	8.861	61.478	54.548	9.702	198.386	133.769	-20.881
1500	8.932	62.092	55.030	10.592	198.148	129.161	-18.818
1600	9.005	62.670	55.490	11.489	197.905	124.568	-17.014
1700	9.078	63.218	55.929	12.393	197.661	119.955	-15.426
1800	9.151	63.739	56.348	13.304	197.414	115.434	-14.015
1900	9.225	64.2[illegible]6	56.750	14.223	197.[illegible]69	110.886	-12.754
2000	9.297	64.711	57.137	15.149	196.92[illegible]	106.346	-11.620
2100	9.369	65.167	57.508	16.082	196.684	101.825	-10.597
2200	9.439	65.604	57.866	17.023	196.443	97.317	-9.667
2300	9.508	66.025	58.212	17.970	196.206	92.807	-8.818
2400	9.574	66.431	58.546	18.924	195.970	88.325	-8.043
2500	9.639	66.823	58.869	19.885	195.739	83.843	-7.329
2600	9.701	67.203	59.183	20.852	195.508	79.373	-6.672
2700	9.761	67.570	59.487	21.825	195.281	74.906	-6.063
2800	9.818	67.926	59.782	22.804	195.058	70.451	-5.499
2900	9.873	68.271	60.069	23.788	194.834	66.007	-4.974
3000	9.925	68.607	60.348	24.778	194.614	61.563	-4.485
3100	9.975	68.933	60.619	25.773	194.397	57.136	-4.028
3200	10.022	69.251	60.884	26.773	194.181	52.714	-3.600
3300	10.067	69.560	61.143	27.778	193.966	48.289	-3.198
3400	10.110	69.861	61.395	28.787	193.753	43.884	-2.821
3500	10.151	70.1[illegible]	61.641	29.800	193.540	39.473	-2.465
3600	10.189	70.442	61.881	30.817	193.3[illegible]	35.082	-2.130
3700	10.226	70.721	62.117	31.838	193.[illegible]	30.684	-1.812
3800	10.260	70.995	62.347	32.862	19[illegible]	26.296	-1.512
3900	10.293	71.262	62.572	33.890	192.6[illegible]	21.910	-1.228
4000	10.323	71.523	62.793	34.921	192.489	17.536	-0.958
4100	10.353	71.778	63.009	35.955	192.279	13.161	-0.702
4200	10.380	72.026	63.221	36.991	192.067	8.803	-0.458
4300	10.406	72.273	63.428	38.031	191.855	4.438	-0.226
4400	10.431	72.51[illegible]	63.63[illegible]	39.073	191.643	0.075	-0.004
4500	10.454	72.747	63.83[illegible]	40.117	191.429	-4.275	0.208
4600	10.476	72.978	64.029	41.164	191.214	-8.620	0.410
4700	10.497	73.20[illegible]	64.22[illegible]	42.212	191.[illegible]99	-12.958	0.603
4800	10.517	73.42[illegible]	64.411	43.263	190.779	-17.299	0.788
4900	10.536	73.64[illegible]	64.598	44.316	190.560	-21.634	0.965
5000	10.554	73.85[illegible]	64.781	45.371	190.339	-25.965	1.135
5100	10.571	74.06[illegible]	64.961	46.427	190.113	-30.284	1.298
5200	10.587	74.270	65.139	47.485	189.887	-34.606	1.454
5300	10.603	74.472	65.31[illegible]	48.545	189.659	-38.923	1.605
5400	10.618	74.671	65.485	49.606	189.429	-43.227	1.749
5500	10.633	74.866	65.654	50.669	189.193	-47.542	1.889
5600	10.647	75.058	65.820	51.733	188.957	-51.850	2.023
5700	10.661	75.247	65.984	52.799	188.717	-56.139	2.152
5800	10.674	75.433	66.146	53.866	188.474	-60.442	2.278
5900	10.687	75.616	66.305	54.934	188.228	-64.735	2.398
6000	10.700	75.796	66.462	56.004	187.978	-69.018	2.514

15 September 1962 — GHW

DIATOMIC CARBON (C_2) (IDEAL MOLECULAR GAS) gfw = 24.022

ΔH°_{f0} = 196.636 Kcal gfw^{-1}

$\Delta H^\circ_{f298.15}$ = 198.660 Kcal gfw^{-1}

Ground State Configuration $^1\Sigma_g{}^+$

$S^\circ_{298.15}$ = 47.630 cal deg K^{-1} gfw^{-1}

$H^\circ_{298.15}-H^\circ_0$ = 2.528 Kcal gfw^{-1}

Spectroscopic constants from Clementi,[1] for 13 electronic states were used. See volume 1, this study (section IVA4c) for details.

Heat of Formation

Based on data of Drowart, et al[2].

Heat Capacity and Entropy

Calculated on diatomic gas computer program.

References

1. Clementi, E., Astrophys. J. 133, 303 (1961).

2. Drowart, J., et al, J. Chem. Phys. 31, 1131 (1959).

TABLE 122

TRIMOLYBDENUM DICARBIDE CONDENSED PHASE C_2Mo_3

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p Solid Mo from 0° to 2890°K, Liquid Mo from 2890° to 4965°K, Gaseous Mo from 4965° to 6000°K, Solid C; Solid Mo_3C_2 from 0° to 2923°K.

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	---	---	---	---	---	---	---
298.15	24.639	23.710	23.710	0.000	-13.970	-14.120	10.350
300	24.741	23.863	23.710	0.046	-13.965	-14.121	10.286
400	28.516	31.564	24.735	2.732	-13.523	-14.236	7.778
500	30.539	38.164	26.778	5.693	-13.024	-14.464	6.322
600	31.873	43.856	29.161	8.817	-12.522	-14.808	5.393
700	32.882	48.848	31.624	12.057	-12.037	-15.226	4.754
800	33.717	53.295	34.060	15.388	-11.544	-15.716	4.293
900	34.452	57.309	36.424	18.797	-11.059	-16.266	3.950
1000	35.123	60.975	38.698	22.276	-10.572	-16.871	3.687
1100	35.754	64.352	40.879	25.820	-10.114	-17.525	3.482
1200	36.357	67.489	42.967	29.426	-9.680	-18.216	3.317
1300	36.940	70.422	44.968	33.091	-9.273	-18.946	3.185
1400	37.509	73.181	46.885	36.814	-8.882	-19.704	3.076
1500	38.068	75.788	48.726	40.593	-8.481	-20.492	2.986
1600	38.618	78.262	50.495	44.427	-8.127	-21.300	2.909
1700	39.163	80.620	52.199	48.316	-[illegible] 807	-22.138	2.846
1800	39.702	82.874	53.841	52.259	-7.524	-22.988	2.791
1900	40.238	85.034	55.426	56.256	-7.283	-23.854	2.744
2000	40.770	87.112	56.959	60.307	-7.087	-24.736	2.703
2100	41.300	89.114	58.442	64.410	-6.942	-25.619	2.666
2200	41.828	91.047	59.881	68.567	-6.856	-26.510	2.633
2300	42.354	92.918	61.277	72.776	-6.828	-27.407	2.604
2400	42.879	94.732	62.633	77.038	-6.867	-28.298	2.577
2500	43.403	96.493	63.952	81.352	-6.979	-29.182	2.551
2600	43.925	98.206	65.237	85.718	-7.171	-30.074	2.528
2700	44.447	99.873	66.489	90.137	-7.441	-30.950	2.505
2800	44.968	101.499	67.711	94.608	-7.796	-31.809	2.483
2890	45.436	102.929	68.785	98.676	-8.198	-32.573	2.463
2890	45.436	102.929	68.785	98.676	-28.148	-32.573	2.463
2900	45.488	103.086	68.903	99.130	-28.116	-32.582	2.455
2923	45.607	103.446	69.174	100.178	-28.036	-32.607	2.438

15 September 1963 DFA

TRIMOLYBDENUM DICARBIDE (Mo_3C_2) (CONDENSED PHASE) gfw = 311.87

$\Delta H^\circ_{f298.15} = -13.97$ kcal gfw^{-1} $\quad$ $S^\circ_{298.15} = 23.71$ cal deg K^{-1} gfw^{-1}

$T_m = 2923°K$

$C^\circ_p = 30.65 + (5.14 \times 10^{-3})T - (6.71 \times 10^5)T^{-2}$ cal deg K^{-1} gfw^{-1} $\quad 298.15°K \leq T \leq 2923°K$

Structure

Mo_3C_2 has a hexagonal structure (a = 3.00 A c = 14.61 A) with a high-temperature cubic form (a = 4.26 A).

Heat of Formation

The heat of formation was calculated from the free-energy functions and the free energy at 1700°K. The free energy at 1700°K was calculated from the disproportionation reaction of Mo_3C_2 to Mo_2C and C.

Heat Capacity and Entropy

The heat-capacity equation was estimated by Krikorian[2]. The entropy was calculated from an estimated $S^\circ_{298.15}$, Mo_3C_2 of 0.5 e.u.

Melting and Vaporization

The melting temperature was determined by Nowotny.[1]

References

1. Nowotny, H., E. Parthe, R. Kieffer and F. Benesovsky, Monat Chem 85, 255 (1954).

2. Krikorian, O., Estimation of High Temperature Heat Capacities of Carbides, UCRL-6785 (1962).

TABLE 123

THORIUM DICARBIDE CONDENSED PHASE C_2Th

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Th from 0° to 2028°K, Liquid Th from 2028° to 5060°K, Gaseous Th from 5060° to 6000°K, Solid C, Solid ThC_2 from 0° to 2928°K.

T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
	cal/°K/gfw			kcal/gfw			
0							
298.15	10.249	15.100	15.100	0.000	-46.600	-46.487	34.074
300	10.289	15.164	15.100	0.019	-46.601	-46.487	33.864
400	11.762	18.352	15.525	1.131	-46.648	-46.442	25.374
500	12.552	21.068	16.369	2.350	-46.758	-46.379	20.271
600	13.072	23.406	17.352	3.632	-46.950	-46.288	16.860
700	13.465	25.451	18.366	4.960	-47.215	-46.157	14.410
800	13.791	27.271	19.367	6.323	-47.538	-45.985	12.562
900	14.077	28.912	20.338	7.717	-47.912	-45.768	11.114
1000	14.336	30.409	21.271	9.138	-48.324	-45.509	9.946
1100	14.583	31.767	22.166	10.584	-48.778	-45.206	8.981
1200	14.818	33.066	23.021	12.054	-49.275	-44.860	8.170
1300	15.04[illegible]	34.261	23.840	13.547	-49.823	-44.469	7.476
1400	15.266	35.384	24.625	15.063	-50.420	-44.034	6.874
1500	15.484	36.445	25.378	16.600	-51.082	-43.558	6.346
1600	15.698	37.451	26.102	18.159	-51.817	-43.032	5.878
1633	15.768	37.772	26.334	18.679	-52.076	-42.846	5.734
1633	15.768	37.772	26.334	18.679	-52.729	-42.846	5.734
1700	15.909	38.409	26.798	19.740	-53.175	-42.432	5.455
1800	16.119	39.3[illegible]5	27.468	21.341	-53.832	-41.780	5.072
1900	16.727	40.202	28.116	22.964	-54.473	-41.094	4.727
2000	16.534	41.044	28.741	24.607	-55.100	-40.374	4.412
2028	16.592	41.275	28.913	25.070	-55.273	-40.167	4.328
2028	16.592	41.275	28.913	25.070	-59.126	-40.167	4.328
2100	16.741	41.856	29.346	26.270	-59.564	-39.483	4.109
2200	16.946	42.640	29.933	27.955	-60.161	-38.513	3.826
2300	17.150	43.397	30.502	29.660	-60.740	-37.520	3.565
2400	17.35[illegible]	44.132	31.055	31.385	-61.305	-36.496	3.323
2500	17.[illegible]	44.844	31.592	33.130	-61.852	-35.450	3.099
2600	17.761	45.537	32.115	34.896	-62.384	-34.383	2.890
2700	17.964	46.21[illegible]	32.625	36.683	-62.897	-33.300	2.695
2800	18.167	46.868	33.122	38.489	-63.393	-32.191	2.513
2900	18.36[illegible]	47.509	33.607	40.316	-63.874	-31.070	2.341
2928	18.4[illegible]	47.686	33.741	40.831	-64.005	-30.754	2.295

THORIUM DICARBIDE (ThC_2) (CONDENSED PHASE) gfw = 256.072

$\Delta H^\circ_{f298.15}$ = -46.6 kcal gfw^{-1} $S^\circ_{298.15}$ = 15.1 ± 3.0 cal degK^{-1} gfw^{-1}

T_m = 2928 ± 25 °K

C°_p = (12.60 ± 1.16) + (2.00 ± 0.18) 10^{-3} T -(2.63 ± 0.20) x $10^5 T^{-2}$ cal deg K^{-1} gfw^{-1}

298 °K ≤ T ≤ 2928°K

Heat of Formation

Computed indirectly; see volume 1, this study (section IVB29. 2).

Heat Capacity and Entropy

Empirical equation developed by Krikorian.[1]

Melting and Vaporization

Melting point from Wilhelm and Chiotti.[2]
Vaporization of Jackson and co-workers.[3]

References

1. Krikorian, O. H., UCRL 2888
2. Wilhelm, H., and Chiotti, P., Trans. Am. Soc. Met. 42, 1295 (1950).
3. Jackson. D. D., G. W. Barton, O. H. Krikorian, and R. S. Newbury, UCRL 6701 (1962).

THORIUM DICARBIDE (ThC_2) (CONDENSED PHASE) GFW = 256.072

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal/gfw)	ΔH_f (Kcal/gfw)	ΔF_f (Kcal/gfw)	Log K_p
298.15	± 0.989	±3.000	±3.000	± 0.000			
500	± 1.170	±3.564	±3.120	± 0.222			
1000	± 1.320	±4.428	±3.579	± 0.849			
1500	± 1.421	±4.982	±3.959	± 1.535			
2000	± 1.515	±5.404	±4.270	± 2.269			
2500	± 1.607	±5.752	±4.532	± 3.050			
2928	± 1.685	±6.012	±4.730	± 3.754			

THORIUM DICARBIDE | IDEAL MOLECULAR GAS | C_2Th

Reference State for Calculating ΔH_f°, ΔF_f°, and Log Kp: Solid Th from 0° to 2028°K, Liquid Th from 2028° to 5060°K, Gaseous Th from 5060° to 6000°K, Solid C; Gaseous ThC_2.

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-2.469	162.791	162.791	INFINITE
298.15	10.255	61.136	61.136	0.000	163.200	149.587	-109.645
300	10.271	61.199	61.136	0.019	163.199	149.503	-108.907
400	10.876	64.245	61.547	1.079	163.100	144.949	-79.193
500	11.312	66.720	62.342	2.189	162.881	140.434	-61.381
600	11.731	68.819	63.251	3.341	162.559	135.973	-49.526
700	12.159	70.659	64.180	4.535	162.160	131.573	-41.077
800	12.588	72.311	65.095	5.773	161.712	127.233	-34.757
900	13.003	73.818	6[illegible].982	7.053	161.224	122.952	-29.855
1000	13.389	75.208	66.836	8.372	160.710	118.726	-25.946
1100	13.736	76.501	67.656	9.729	160.167	114.555	-22.759
1200	14.040	77.710	68.444	11.118	159.589	110.432	-20.112
1300	14.296	78.844	69.201	12.535	158.965	106.361	-17.880
1400	14.505	79.911	69.928	13.976	158.293	102.342	-15.976
1500	14.668	80.918	70.628	15.435	157.553	98.367	-14.331
1600	14.790	81.869	71.301	16.908	156.732	94.450	-12.901
1633	14.822	82.171	71.517	17.397	15[illegible].442	93.170	-12.469
1633	14.822	82.171	71.517	17.397	155.789	93.170	-12.469
1700	14.875	82.768	71.949	18.392	155.277	90.612	-11.648
1800	14.928	83.620	72.574	19.882	154.509	86.830	-10.542
1900	14.953	84.428	73.177	21.376	153.739	83.090	-9.557
2000	14.956	85.195	73.759	22.872	152.965	79.390	-8.675
2028	14.953	85.403	73.918	23.291	152.748	78.363	-8.444
2028	14.953	85.403	73.918	23.291	148.895	78.363	-8.444
2100	14.941	85.924	74.321	24.367	148.333	75.869	-7.895
2200	14.912	86.619	74.864	25.860	147.544	72.439	-7.196
2300	14.871	87.281	75.390	27.349	146.749	69.038	-6.560
2400	14.823	87.913	75.898	28.834	145.944	65.681	-5.981
2500	14.768	88.517	76.391	30.313	145.131	62.352	-5.451
2600	14.710	89.095	76.869	31.787	144.307	59.057	-4.964
2700	14.650	89.649	77.332	33.255	143.475	55.791	-4.516
2800	14.588	90.180	77.781	34.717	142.635	52.564	-4.103
2900	14.526	90.691	78.218	36.173	141.783	49.358	-3.720
3000	14.464	91.183	78.642	37.622	140.922	46.185	-3.364
3100	14.403	91.656	79.054	39.066	140.054	43.041	-3.034
3200	14.344	92.112	79.455	40.503	13[illegible].175	39.930	-2.727
3300	14.286	92.553	79.845	41.934	138.[illegible]16	36.836	-2.439
3400	14.231	92.978	80.225	43.360	137.[illegible]	33.782	-2.171
3500	14.177	93.390	80.596	44.781	136.485	30.743	-1.920
3600	14.126	93.789	80.957	46.196	1[illegible]5.572	27.736	-1.684
3700	14.077	94.175	81.309	47.606	134.650	24.753	-1.462
3800	14.030	94.550	81.652	49.011	133.721	21.794	-1.253
3900	13.985	94.914	81.988	50.412	132.784	18.857	-1.057
4000	13.942	95.267	82.315	51.808	131.840	15.952	-0.872
4100	13.901	95.611	82.635	53.200	130.888	13.066	-0.696
4200	13.862	95.946	82.948	54.589	129.929	10.207	-0.531
4300	13.825	96.271	83.254	55.973	128.961	7.364	-0.374
4400	13.790	96.589	83.554	57.354	127.988	4.545	-0.226
4500	13.757	96.898	83.847	58.731	127.007	1.754	-0.085
4600	13.725	97.200	84.134	60.105	126.019	-1.020	0.048
4700	13.694	97.495	84.415	61.476	125.026	-3.772	0.175
4800	13.666	97.783	84.691	62.844	124.024	-6.499	0.296
4900	13.638	98.065	84.961	64.209	123.017	-9.206	0.411
5000	13.612	98.340	85.225	65.572	122.004	-11.895	0.520
5060.26	13.597	98.503	85.383	66.392	121.389	-13.504	0.583
5060.26	13.597	98.503	85.383	66.392	-1.376	-13.504	0.583
5100	13.587	98.609	85.485	66.932	-1.717	13.597	0.583
5200	13.563	98.873	85.740	68.289	-2.581	-13.824	0.581
5300	13.541	99.131	85.990	69.644	-3.455	-14.027	0.578
5400	13.519	99.384	86.236	70.997	-4.339	-14.217	0.575
5500	13.499	99.632	86.477	72.348	-5.234	-14.395	0.572
5600	13.479	99.875	86.714	73.697	-6.136	-14.555	0.568
5700	13.461	100.113	86.947	75.044	-7.049	-14.691	0.563
5800	13.443	100.347	87.176	76.389	-7.970	-14.814	0.558
5900	13.426	100.577	87.402	77.733	-8.899	-14.933	0.553
6000	13.410	100.802	87.623	79.075	-9.835	-15.030	0.547

15 September 1963 MBP

THORIUM DICARBIDE (ThC_2) (IDEAL MOLECULAR GAS) gfw = 256.072

ΔH°_{f0} = 162.791 kcal gfw^{-1}

$\Delta H^\circ_{f298.15}$ = 163.2 kcal gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 2.469 kcal gfw^{-1}

$S^\circ_{298.15}$ = 61.136 cal degK^{-1} gfw^{-1}

Vibrational Levels and Multiplicities

ω, cm^{-1}	ω , cm^{-1}
592	1756
399	

Bond lengths and angles:

Th-C distance = 1.90 A

C-C distance = 1.31 A

Electronic Contribution First ten levels for Th III[1]

Computed from vaporization data of Jackson & co-workers[2] by third law method

Heat Capacity and Entropy

Computed using the spectroscopic data given above.

References

1. De Bruin, T. L., P. F. Klinkenbert, and P. Schuurmans, Zeit. Phys. 118,58 (1941).
2. Jackson, D. D., G. W. Barton, O. J. Krikorian, and R. S. Newbury, UCRL 6701 (April 1962).

TRIATOMIC CARBON IDEAL MOLECULAR GAS C_3

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p
Solid Graphite from 0° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.319	187.377	187.377	INFINITE
298.15	9.388	50.689	50.689	0.000	188.940	175.043	-128.304
300	9.407	50.748	50.690	0.017	188.945	174.956	-127.449
400	10.311	53.583	51.070	1.005	189.195	170.252	-93.017
500	11.030	55.964	51.817	2.073	189.306	166.001	-72.555
600	11.623	58.029	52.684	3.207	189.306	160.737	-58.546
700	12.115	59.859	53.581	4.395	189.219	155.982	-48.697
800	12.524	61.504	54.470	5.627	189.074	151.242	-41.315
900	12.862	62.999	55.336	6.897	188.883	146.525	-35.579
1000	13.141	64.369	56.172	8.198	188.666	141.828	-30.995
1100	13.373	65.633	56.975	9.524	188.423	137.158	-27.249
1200	13.566	66.805	57.746	10.871	188.162	132.508	-24.132
1300	13.727	67.898	58.485	12.236	187.880	127.881	-21.498
1400	13.862	68.920	59.195	13.615	187.591	123.278	-19.244
1500	13.977	69.880	59.875	15.008	187.292	118.694	-17.293
1600	14.074	70.786	60.529	16.410	186.984	114.131	-15.589
1700	14.158	71.641	61.158	17.822	18[illegible].674	109.589	-14.088
1800	14.230	72.453	61.763	19.241	186.356	105.064	-12.756
1900	14.292	73.224	62.346	20.668	186.037	100.556	-11.566
2000	14.347	73.958	62.908	22.100	185.714	96.064	-10.497
2100	14.394	74.659	63.451	23.537	185.390	91.589	-9.531
2200	14.436	75.330	63.976	24.978	185.058	87.133	-8.655
2300	14.473	75.973	64.484	26.424	184.728	82.683	-7.856
2400	14.506	76.589	64.976	27.873	184.392	78.257	-7.126
2500	14.536	77.182	65.452	29.325	184.056	73.843	-6.455
2600	14.562	77.753	65.914	30.780	183.714	69.441	-5.837
2700	14.586	78.303	66.363	32.237	183.371	65.051	-5.265
2800	14.607	78.834	66.799	33.697	183.028	60.679	-4.736
2900	14.626	79.346	67.223	35.159	182.678	56.312	-4.244
3000	14.644	79.843	67.635	36.622	182.326	51.960	-3.785
3100	14.660	80.323	68.037	38.087	181.973	47.616	-3.356
3200	14.674	80.789	68.428	39.554	181.616	43.296	-2.957
3300	14.687	81.240	68.810	41.022	181.254	38.970	-2.581
3400	14.700	81.679	69.182	42.491	180.890	34.670	-2.228
3500	14.711	82.105	69.545	43.962	180.522	30.373	-1.896
3600	14.721	82.520	69.899	45.434	180.1[illegible]2	26.089	-1.584
3700	14.731	82.923	70.246	46.906	179.[illegible]6	21.815	-1.289
3800	14.739	83.316	70.585	48.380	179.399	17.548	-1.009
3900	14.748	83.699	70.916	49.854	179.016	13.291	-0.745
4000	14.755	84.073	71.241	51.329	1[illegible]8.631	9.048	-0.494
4100	14.762	84.437	71.558	52.805	178.241	4.813	-0.257
4200	14.769	84.793	71.869	54.282	177.846	0.592	-0.031
4300	14.775	85.1[illegible]1	72.173	55.759	177.445	-3.625	0.184
4400	14.781	85.480	72.472	57.237	177.042	-7.836	0.389
4500	14.786	85.813	72.765	58.715	176.633	-12.033	0.584
4600	14.791	86.138	73.052	60.194	176.219	-16.220	0.771
4700	14.796	86.456	73.334	61.673	175.802	-20.398	0.948
4800	14.800	86.767	73.610	63.153	175.377	-24.562	1.118
4900	14.804	87.073	73.882	64.633	174.949	-28.729	1.281
5000	14.808	87.372	74.149	66.114	174.516	-32.885	1.437
5100	14.812	87.665	74.411	67.595	174.074	-37.021	1.586
5200	14.815	87.953	74.669	69.076	173.629	-41.153	1.730
5300	14.819	88.235	74.922	70.558	173.179	-45.283	1.867
5400	14.822	88.512	75.171	72.040	172.723	-49.394	1.999
5500	14.825	88.784	75.416	73.522	172.258	-53.504	2.126
5600	14.827	89.051	75.657	75.005	171.791	-57.618	2.249
5700	14.830	89.313	75.895	76.488	171.315	-61.703	2.366
5800	14.833	89.571	76.128	77.971	170.833	-65.778	2.478
5900	14.835	89.825	76.358	79.454	170.345	-69.862	2.588
6000	14.837	90.075	76.585	80.938	169.849	-73.938	2.693

15 September 1962 CHW

TRIATOMIC CARBON (C_3) (IDEAL MOLECULAR GAS) gfw = 36.033

ΔH°_{f0} = 187.377 Kcal gfw^{-1}

$\Delta H^\circ_{f298.15}$ = 188.940 Kcal gfw^{-1}

Point Group $D_{\infty h}$

$S^\circ_{298.15}$ = 50.689 cal deg K^{-1} gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 2.319 Kcal gfw^{-1}

Vibrational levels and multiplicities

ω, cm^{-1}	ω, cm^{-1}
1300 (1)	2200 (1)
550 (2)	

Bond lengths and angles:

C-C distance = 1.281 A

C-C-C Angle = 180 deg

Moment of inertia: = 65.448 x 10^{-40} gcm^2 $\sigma = 2$

Heat of Formation

Based on data of Drowart, et al[1]

Heat Capacity and Entropy

Calculated on polyatomic gas computer program.

Reference

1. Drowart, J., et al, J. Chem. Phys. 31, 1131 (1959).

CALCIUM — REFERENCE STATE — Ca

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p. Solid Ca from 0° to 1123°K, Liquid Ca from 1123° to 1765°K, Gaseous Ca from 1765° to 6000°K.

T, °K	cal/°K gfw C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	Kcal/gfw $H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.375			
298.15	6.280	9.950	9.950	0.000			
300	6.287	9.989	9.950	0.012			
400	6.647	11.847	10.201	0.658			
500	7.008	13.369	10.687	1.341			
600	7.368	14.678	11.245	2.060			
700	7.729	15.841	11.820	2.815			
737	7.862	16.243	12.032	3.103			
737	7.665	16.568	12.032	3.343			
800	8.083	17.214	12.415	3.839			
900	8.775	18.205	13.004	4.682			
1000	9.490	19.167	13.572	5.595			
1100	10.221	20.105	14.123	6.580			
1123	10.390	20.319	14.248	6.817			
1123	7.400	22.162	14.248	8.887			
1200	7.400	22.653	14.772	9.457			
1300	7.400	23.245	15.401	10.197			
1400	7.400	23.793	15.981	10.937			
1500	7.400	24.304	16.519	11.677			
1600	7.400	24.781	17.021	12.417			
1700	7.400	25.230	17.491	13.157			
1765	7.400	25.504	17.777	13.638			
1765	4.980	45.827	17.777	49.509			
1800	4.982	45.927	18.325	49.683			
1900	4.993	46.197	19.785	50.182			
2000	5.008	46.453	21.112	50.682			
2100	5.030	46.698	22.325	51.184			
2200	5.061	46.933	23.438	51.689			
2300	5.101	47.158	24.464	52.197			
2400	5.153	47.377	25.415	52.709			
2500	5.219	47.588	26.297	53.228			
2600	5.300	47.794	27.120	53.753			
2700	5.397	47.996	27.889	54.288			
2800	5.511	48.1[illegible]4	28.611	54.833			
2900	5.644	48.390	29.290	55.391			
3000	5.796	48.584	29.930	55.963			
3100	5.968	48.777	30.535	56.551			
3200	6.160	48.969	31.107	57.157			
3300	6.371	49.162	31.652	57.783			
3400	6.601	49.355	32.169	58.432			
3500	6.849	49.550	32.663	59.104			
3600	7.115	49.747	33.135	59.802			
3700	7.397	49.946	33.587	60.528			
3800	7.692	50.147	34.020	61.282			
3900	8.001	50.351	34.436	62.067			
4000	8.320	50.557	34.836	62.883			
4100	8.648	50.767	35.223	63.731			
4200	8.983	50.979	35.595	64.613			
4300	9.323	51.194	35.955	65.528			
4400	9.666	51.413	36.305	66.477			
4500	10.010	51.634	36.643	67.461			
4600	10.353	51.858	36.971	68.479			
4700	10.694	52.084	37.290	69.532			
4800	11.030	52.313	37.601	70.618			
4900	11.362	52.543	37.903	71.737			
5000	11.687	52.776	38.198	72.890			
5100	12.004	53.011	38.487	74.075			
5200	12.313	53.247	38.768	75.290			
5300	12.612	53.484	39.043	76.537			
5400	12.902	53.723	39.313	77.813			
5500	13.181	53.967	39.577	79.117			
5600	13.450	54.202	39.836	80.448			
5700	13.708	54.442	40.090	81.806			
5800	13.954	54.683	40.340	83.190			
5900	14.190	54.923	40.585	84.597			
[illegible]	14.414	[illegible]	40.826	86.027			

May 1962 RCF

CALCIUM (Ca) (REFERENCE STATE) gfw = 40.08

$0^{\circ}K$ to $1123^{\circ}K$ Crystal

$1123^{\circ}K$ to $1765^{\circ}K$ Liquid

$1765^{\circ}K$ to $6000^{\circ}K$ Ideal Monatomic Gas

$\Delta H^{o}_{f0} = 0$

$\Delta H^{o}_{f298.15} = 0$

$\Delta H^{o}_{s298.15} = 42.220$ kcal gfw^{-1}

$S^{o}_{298.15} = 9.95$ cal degK^{-1}gfw^{-1}

$T_t = 737^{o}K$

$\Delta H_t = 0.240$ kcal gfw^{-1}

$T_m = 1123^{o}K$

$\Delta H_m = 2.070$ kcal gfw^{-1}

$T_b = 1765^{o}K$

$\Delta H_v = 35.871$ kcal gfw^{-1}

$H^{o}_{298.15} - H^{o}_{0} = 1.375$ kcal gfw^{-1}

$C^{o}_{p} = 5.205 + 3.605\times10^{-3}T$ cal deg K^{-1} gfw^{-1} $\quad 298.15^{o}K \le T \le 737^{o}K$

$C^{o}_{p} = 1.50 + 7.74\times10^{-3}T + 2.5\times10^{5}T^{-2}$ cal degK^{-1}gfw^{-1} $\quad 737^{o}K \le T \le 1123^{o}K$

$C^{o}_{p} = 7.400$ cal degK^{-1}gfw^{-1} $\quad 1123^{o}K \le T \le 1765^{o}K$

Structure

Low-temperature form has an f. c. c. structure, above $737^{o}K$, Ca has a b. c. c. structure.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Low-temperature data from Kelley and King.[1] High-temperature data based on Jauch,[2] and Eastman, Williams, and Young.[3]

Melting

Melting point from Kubaschewski *et al.*[4]

Vaporization

Average of several determinations.

Further details by Barriault *et al.*[5]

References

1. Kelley, K. K. and E. G. King, U. S. Bur. Mines, Bull. 592 (1961).
2. Jauch, R., Diplomarbeit, Techn. Hochschule, Stuttgart (1946).
3. Eastman, E.D., A. M. Williams, and T. F. Young, J. Am. Chem. Soc. 46, 1178 (1924).
4. Kubaschewski, O. et al, Z. Elektrochem. 54, 275 (1950).
5. Barriault, R. J. et al, ASD TR 61-260 (May 1962), Pt. 1.

CALCIUM (Ca) (REFERENCE STATE) GFW = 40.08

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^{o}_{p} (cal/°K gfw)	S^{o}_{T} (cal/°K gfw)	$-(F^{o}_{T} - H^{o}_{298})/T$ (cal/°K gfw)	$H^{o}_{T} - H^{o}_{298}$ (Kcal gfw)	ΔH_f (Kcal gfw)	ΔF_f (Kcal gfw)	Log K_p
298.15	±0.100	±0.100	±0.100	±0.000			
737	±0.200	±0.140	±0.120	±0.020			
737	±0.300	±0.230	±0.120	±0.080			
1123	±1.000	±0.370	±0.180	±0.220			
1123	±0.500	±0.460	±0.180	±0.320			
1765	±1.500	±0.690	±0.320	±0.640			
1765	±0.000	±0.002					
2000	±0.000	±0.002					
3000	±0.001	±0.002					
4000	±0.002	±0.002					
5000	±0.003	±0.003					
6000	±0.003	±0.003					

TABLE 127

CALCIUM — IDEAL MONATOMIC GAS — Ca

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ca from 0° to 1123°K, Liquid Ca from 1123° to 1765°K, Gaseous Ca from 1765° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.481	42.114	42.114	INFINITE
298.15	4.968	36.993	36.993	0.000	42.220	34.157	-25.037
300	4.968	37.024	36.993	0.009	42.217	34.107	-24.846
400	4.968	38.453	37.188	0.506	42.068	31.426	-17.170
500	4.968	39.562	37.556	1.003	41.882	28.786	-12.582
600	4.968	40.468	37.968	1.500	41.660	26.186	-9.538
700	4.968	41.233	38.381	1.996	41.401	23.627	-7.376
737	4.968	41.489	38.531	2.180	41.297	22.690	-6.728
737	4.968	41.489	38.531	2.180	41.057	22.690	-6.728
800	4.968	41.897	38.780	2.493	40.874	21.127	-5.771
900	4.968	42.482	39.160	2.990	40.528	18.679	-4.536
1000	4.968	43.005	39.519	3.487	40.112	16.273	-3.556
1100	4.968	43.479	39.857	3.984	39.624	13.913	-2.764
1123	4.968	43.582	39.933	4.098	39.501	13.376	-2.603
1123	4.968	43.582	39.933	4.098	37.431	13.376	-2.603
1200	4.968	43.911	40.178	4.481	37.244	11.733	-2.137
1300	4.968	44.309	40.480	4.977	37.[illegible]30	9.616	-1.617
1400	4.969	44.677	40.767	5.474	36.757	7.518	-1.174
1500	4.970	45.020	41.039	5.971	36.5[illegible]4	5.438	-0.792
1600	4.972	45.341	41.298	6.468	36.271	3.375	-0.461
1700	4.976	45.642	41.545	6.966	36.029	1.327	-0.171
1765	4.980	45.827	41.696	7.289	35.871	0.000	0.000
1765	4.980	45.827	41.696	7.289			
1800	4.982	45.927	41.781	7.463			
1900	4.993	46.197	42.006	7.962			
2000	5.008	46.453	42.222	8.462			
2100	5.036	46.698	42.429	8.964			
2200	5.061	46.933	42.629	.469			
2300	5.101	47.158	42.821	9.977			
2400	5.153	47.377	43.006	10.489			
2500	5.219	47.588	43.185	11.008			
2600	5.300	47.794	43.358	11.533			
2700	5.397	47.996	43.527	12.068			
2800	5.521	48.194	43.690	12.613			
2900	5.644	48.390	43.848	13.171			
3000	5.796	48.584	44.003	13.743			
3100	5.968	48.777	44.154	14.331			
3200	6.160	48.969	44.301	4.937			
3300	6.371	49.162	44.446	15.563			
3400	6.603	49.355	44.587	16.212			
3500	6.849	49.550	44.726	16.884			
3600	7.115	49.747	44.863	17.582			
3700	7.397	49.946	44.998	18.308			
3800	7.692	50.147	45.131	19.062			
3900	8.001	50.351	45.262	19.847			
4000	8.320	50.557	45.392	20.663			
4100	8.648	50.767	45.520	21.511			
4200	8.983	50.979	45.648	22.393			
4300	9.323	51.194	45.774	23.308			
4400	9.666	51.413	45.900	24.257			
4500	10.010	51.634	46.025	25.241			
4600	10.353	51.858	46.149	26.259			
4700	10.694	52.084	46.273	27.312			
4800	11.030	52.313	46.396	28.398			
4900	11.362	52.543	46.519	29.517			
5000	11.687	52.776	46.642	30.670			
5100	12.004	53.011	46.765	31.855			
5200	12.313	53.247	46.887	33.070			
5300	12.612	53.484	47.009	34.317			
5400	12.902	53.723	47.132	35.593			
5500	13.181	53.962	47.254	36.897			
5600	13.450	54.202	47.376	38.228			
5700	13.708	54.442	47.497	39.586			
5800	13.954	54.683	47.619	40.970			
5900	14.190	54.923	47.741	42.377			
6000	14.414	55.164	47.863	43.807			

May 1962 — RCF

CALCIUM (Ca) (IDEAL MONATOMIC GAS) gfw - 40.08

ΔH^o_{f0} = 42.114 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 42.220 kcal gfw^{-1}

Ground State Configuration = $^1S_0$

$S^o_{298.15}$ = 26.993 cal degK^{-1}gfw^{-1}

$H^o_{298.15} - H^o_0$ = 1.481 kcal gfw^{-1}

Electronic Levels and Multiplicities

Energy Levels from Moore.[1]

Heat of Formation

Average of several determinations.

Heat Capacity and Entropy

Calculated on monatomic gas-computer program.

Further details by Barriault et al.[2]

References

1. Moore, C., Atomic Energy Levels, Vol. 1, Nat. Bur. Stds. (1949).
2. Barriault, R. J. et al, ASD TR 61-260 (May 1962), Pt. I.

CALCIUM, MONATOMIC (Ca) (IDEAL GAS) GFW = 40.08

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal °K gfw C^o_p	S_T	$-(F_T - H_{298})/T$	kcal gfw $H_T - H_{298}$	ΔH_f	ΔF_f	Log K_p
298.15	± 0.000	± 0.002	± 0.002	± 0.000	± 0.250	± 0.300	± 0.220
737	± 0.000	± 0.002	± 0.002	± 0.000	± 0.250	± 0.340	± 0.110
737	± 0.000	± 0.002	± 0.002	± 0.000	± 0.250	± 0.340	± 0.110
1123	± 0.000	± 0.002	± 0.002	± 0.000	± 0.450	± 0.450	± 0.088
1123	± 0.000	± 0.002	± 0.002	± 0.000	± 0.550	± 0.450	± 0.088
1765	± 0.000	± 0.002	± 0.002	± 0.000	± 0.870	± 0.830	± 0.100
1765	± 0.000	± 0.002	± 0.002	± 0.000			
2000	± 0.000	± 0.002	± 0.002	± 0.000			
3000	± 0.001	± 0.002	± 0.002	± 0.001			
4000	± 0.002	± 0.002	± 0.002	± 0.002			
5000	± 0.003	± 0.003	± 0.003	± 0.003			
6000	± 0.003	± 0.003	± 0.003	± 0.005			

CALCIUM OXIDE — CONDENSED PHASE — CaO

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ca from 0° to 1123°K, Liquid Ca from 1123° to 1765°K, Gaseous Ca from 1765°K to 4000°K, Gaseous O_2. Solid CaO from 0° to 2860°K, Liquid CaO from 2860° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f (Kcal/gfw)	ΔF_f (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.668	-150.666	-150.666	INFINITE
298.15	10.230	9.561	9.561	0.000	-151.410	-143.988	105.541
300	10.254	9.624	9.561	0.019	-151.410	-143.942	104.857
400	11.120	12.708	9.976	1.093	-151.336	-141.463	77.288
500	11.579	15.243	10.784	2.230	-151.248	-139.005	60.756
600	11.878	17.383	11.710	3.404	-151.171	-136.564	49.741
700	12.101	19.231	12.655	4.603	-151.115	-134.134	41.877
737	12.172	19.856	13.001	5.052	-151.101	-133.237	39.508
737	12.172	19.856	13.001	5.052	-151.341	-133.237	39.508
800	12.283	20.859	13.581	5.822	-151.319	-131.690	35.974
900	12.442	22.315	14.472	7.059	-151.333	-129.236	31.381
1000	12.587	23.634	15.323	8.310	-151.408	-126.778	27.706
1100	12.722	24.840	16.134	9.576	-151.547	-124.309	24.697
1123	12.752	25.103	16.315	9.869	-151.588	-123.739	24.080
1123	12.752	25.103	16.315	9.869	-153.658	-123.739	24.080
1200	12.851	25.952	16.907	10.855	-153.569	-121.690	22.162
1300	12.975	26.986	17.643	12.146	-153.447	-119.039	20.011
1400	13.095	27.952	18.345	13.449	-153.315	-116.397	18.170
1500	13.214	28.859	19.016	14.765	-153.17[illegible]	-113.765	16.575
1600	13.330	29.716	19.658	16.092	-153.026	-111.142	15.181
1700	13.445	30.527	20.274	17.431	-152.869	-108.529	13.952
1764.79	13.519	31.033	20.661	18.307	-152.762	-106.843	13.229
1764.79	13.519	31.033	20.661	18.307	-188.633	-106.843	13.229
1800	13.559	31.299	20.865	18.781	-188.489	-105.219	12.775
1900	13.672	32.035	21.434	20.143	-188.073	-100.605	11.572
2000	13.784	32.739	21.982	21.515	-187.651	-96.011	10.491
2100	13.896	33.415	22.510	22.899	-187.222	-91.439	9.516
2200	14.007	34.064	23.021	24.295	-186.787	-86.888	8.631
2300	14.118	34.689	23.514	25.701	-186.347	-82.359	7.826
2400	14.228	35.292	23.993	27.118	-185.902	-77.845	7.088
2500	14.338	35.875	24.456	28.546	-185.457	-73.354	6.412
2600	14.448	36.439	24.906	29.986	-185.009	-68.878	5.789
2700	14.558	36.987	25.344	31.436	-184.563	-64.422	5.214
2800	14.667	37.518	25.769	32.897	-184.117	-59.979	4.681
2860	14.733	37.870	26.019	33.779	-183.852	-57.327	4.380
2860	16.500	43.844	26.019	50.979	-166.552	-57.327	4.380
2900	16.500	44.073	26.266	51.639	-166.4[illegible]	-55.793	4.204
3000	16.500	44.632	26.869	53.289	-165.[illegible]	-51.989	3.787
3100	16.500	45.173	27.451	54.939	-165.222	-48.203	3.398
3200	16.500	45.697	28.013	56.589	-164.659	-44.442	3.035
3300	16.500	46.205	28.557	58.239	-164.117	-40.690	2.695
3400	16.500	46.697	29.083	59.889	-163.601	-36.961	2.376
3500	16.500	47.176	29.593	61.539	-163.110	-33.242	2.076
3600	16.500	47.641	30.088	63.189	-162.647	-29.537	1.793
3700	16.500	48.093	30.569	64.839	-162.214	-25.845	1.527
3800	16.500	48.533	31.035	66.489	-161.810	-22.164	1.275
3900	16.500	48.961	31.490	68.139	-161.[illegible]40	-18.495	1.036
4000	16.500	49.37[illegible]	31.932	69.789	-161.102	-14.835	0.810
4100	16.500	49.766	32.362	71.439	-160.798	-11.179	0.596
4200	16.500	50.184	32.782	73.089	-160.530	-7.534	0.392
4300	16.500	50.572	33.191	74.739	-160.296	-3.894	0.198
4400	16.500	50.952	33.590	76.389	-160.099	-0.254	0.013
4500	16.500	51.322	33.980	78.039	-159.939	3.375	-0.164
4600	16.500	51.[illegible]	34.361	79.689	-159.815	7.003	-0.333
4700	16.500	52.040	34.734	81.339	-159.728	10.629	-0.494
4800	16.500	52.387	35.098	82.989	-159.678	14.255	-0.649
4900	16.500	52.728	35.454	84.639	-159.663	17.877	-0.797
5000	16.500	53.0[illegible]1	35.803	86.289	-159.687	21.500	-0.940
5100	16.500	53.386	36.145	87.939	-159.747	25.128	-1.077
5200	16.500	53.708	36.479	89.589	-159.842	28.753	-1.208
5300	16.500	54.022	36.807	91.239	-159.975	32.379	-1.335
5400	16.500	54.331	37.129	92.889	-160.145	36.013	-1.457
5500	16.500	54.63[illegible]	37.445	94.539	-160.352	39.649	-1.575
5600	16.500	54.931	37.754	96.189	-160.596	43.287	-1.689
5700	16.500	55.22[illegible]	38.058	97.839	-160.880	46.933	-1.799
5800	16.500	55.510	38.356	99.489	-161.20[illegible]	50.587	-1.906
5900	16.500	55.792	38.6[illegible]0	101.139	-161.574	54.243	-2.009
6000	16.500	56.06[illegible]	38.938	102.78[illegible]	-161.986	57.908	-2.109

15 December 1962 — RCF

CALCIUM OXIDE (CaO) (CONDENSED PHASE) gfw = 56.08

$\Delta H^o_{f298.15} = -151.410$ kcal gfw^{-1} $S^o_{298.15} = 9.561$ cal deg K^{-1}gfw^{-1}

$T_m = 2860^oK$ $\Delta H_m = 17.200$ kcal gfw^{-1}

$H^o_{298.15} - H^o_0 = 1.668$ kcal gfw^{-1}

$C^o_p = 11.67 + 1.08 \times 10^{-3}T - 1.56 \times 10^5 T^{-2}$ cal deg K^{-1}gfw^{-1} $298.15^oK \leq T \leq 2860^oK$

$C^o_p = 16.5$ cal deg K^{-1}gfw^{-1} $2860^oK \leq T \leq 6000^oK$

Structure

An fcc (NaCl) type.

Heat of Formation

Obtained from combustion calorimetry by Huber and Holley.[1]

Heat Capacity and Entropy

Low-temperature data of Nernst and Schwers[2] and Parks and Kelley[3] analyzed by Barriault et al.[4] High-temperature data of Kelley[5] extrapolated to melting point. Liquid heat capacity estimated.

Melting and Vaporization

Heat of fusion estimated.

References

1. Huber, E. J. and C. E. Holley, J. Phys. Chem. 60, 498 (1956).
2. Nernst, W. and F. Schwers, Sitzb. Konig. Preuss. Akad. Wiss. 1, 355 (1914).
3. Parks, G. S. and K. K. Kelley, J. Phys. Chem. 30, 47 (1926).
4. Barriault, R. J. et al, ASD TR 61-260 (May 1962), Pt. 1.
5. Kelley, K. K., U. S. Bur. Mines, Bull. 584 (1960).

CALCIUM OXIDE (CaO) (CONDENSED PHASE) GFW = 56.08

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T (cal/°K gfw)	$-(F^o_T - H^o_{298})/T$ (cal/°K gfw)	$H^o_T - H^o_{298}$ (Kcal gfw)	ΔH_f (Kcal gfw)	ΔF_f (Kcal gfw)	Log K_p
298.15	±0.200	±0.150	±0.150	±0.000	±0.500	±0.570	±0.420
1000	±0.430	±0.290	±0.210	±0.080	±0.760	±0.870	±0.190
2000	±0.930	±0.460	±0.300	±0.330	±1.700	±1.540	±0.170
2860	±1.740	±0.610	±0.370	±0.680	±2.050	±1.860	±0.140
2860	±1.000	±1.100	±0.370	±2.080	±3.450	±1.860	±0.140
4000	±2.000	±1.600	±0.650	±3.790	±5.160	±3.320	±0.180

CALCIUM OXIDE — IDEAL MOLECULAR GAS — CaO

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ca from 0° to 1123°K, Liquid Ca from 1123° to 1765°K, Gaseous Ca from 1765° to 6000°K, Gaseous O_2, Gaseous CaO.

	cal/°K g/m			Kcal/g/m			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-2.117	1.095	1.095	INFINITE
298.15	7.553	54.217	54.217	0.000	0.800	-5.092	3.733
300	7.561	54.263	54.217	0.014	0.795	-5.129	3.736
400	7.952	56.495	54.518	0.791	0.572	-7.070	3.863
500	8.233	58.301	55.100	1.601	0.333	-8.953	3.913
600	8.427	59.820	55.763	2.434	0.069	-10.786	3.928
700	8.564	61.130	56.439	3.284	-0.224	-12.573	3.925
737	8.604	61.572	56.685	3.602	-0.341	-13.222	3.921
737	8.604	61.572	56.685	3.602	-0.581	-13.222	3.921
800	8.663	62.281	57.099	4.146	-0.786	-14.295	3.905
900	8.737	63.305	57.732	5.016	-1.165	-15.960	3.875
1000	8.795	64.229	58.337	5.892	-1.617	-17.582	3.842
1100	8.841	65.069	58.911	6.774	-2.139	-19.153	3.805
1123	8.850	65.253	59.039	6.978	-2.269	-19.508	3.796
1123	8.850	65.253	59.039	6.978	-4.339	-19.508	3.796
1200	8.879	65.840	59.457	7.660	-4.554	-20.540	3.741
1300	8.911	66.552	59.976	8.550	-4.8[illegible]3	-21.862	3.675
1400	8.938	67.[illegible]14	60.469	9.442	-5.113	-23.161	3.615
1500	8.963	67.8[illegible]1	60.940	10.337	-5.393	-24.441	3.561
1600	8.985	68.411	61.389	11.235	-5.673	-25.702	3.511
1700	9.005	68.956	61.818	12.134	-5.956	-26.944	3.464
1764.79	9.017	69.294	62.087	12.720	-6.139	-27.750	3.436
1764.79	9.017	69.294	62.087	12.720	-42.010	-27.750	3.436
1800	9.023	69.471	62.229	13.036	-42.024	-27.465	3.334
1900	9.041	69.960	62.623	13.939	-42.067	-26.654	3.066
2000	9.058	70.424	63.002	14.844	-42.112	-25.842	2.824
2100	9.075	70.866	63.366	15.750	-42.161	-25.027	2.604
2200	9.091	71.289	63.717	1[illegible].659	-42.213	-24.211	2.405
2300	9.108	71.694	64.055	17.569	-42.269	-23.393	2.223
2400	9.125	72.082	64.382	18.480	-42.331	-22.570	2.055
2500	9.142	72.455	64.697	19.394	-42.399	-21.746	1.901
2600	9.161	72.814	65.003	20.309	-42.476	-20.919	1.758
2700	9.180	73.160	65.299	21.226	-42.563	-20.091	1.626
2800	9.200	73.494	65.586	22.145	-42.660	-19.256	1.503
2900	9.221	73.818	65.865	23.066	-42.771	-18.420	1.388
3000	9.244	74.132	66.135	23.989	-42.[illegible]	-17.577	1.280
3100	9.268	74.436	66.399	24.915	-43.03[illegible]	-16.732	1.180
3200	9.293	74.731	66.655	[illegible].843	-43.195	-15.886	1.085
3300	9.320	75.017	66.904	26.773	-43.374	-15.027	0.995
3400	9.349	75.297	67.147	27.707	-43.574	-14.169	0.911
3500	9.378	7[illegible].568	67.385	28.643	-43.797	-13.303	0.831
360[illegible]	9.410	75.834	67.616	29.583	-44.044	-12.428	0.754
3700	9.443	76.092	67.842	30.525	-44.318	-11.547	0.682
3800	9.477	76.345	68.063	31.471	-44.619	-10.659	0.613
3900	9.513	76.593	68.280	32.421	-44.948	-9.767	0.547
4000	9.551	76.835	68.491	33.374	-45.307	-8.862	0.484
4100	9.590	77.072	68.698	34.331	-45.696	-7.945	0.424
4200	9.630	77.304	68.901	35.292	-46.117	-7.025	0.366
4300	9.672	77.532	69.100	36.257	-46.569	-6.093	0.310
4400	9.714	[illegible]7.756	69.295	37.227	[illegible]7.052	-5.144	0.256
4500	9.758	77.975	69.486	38.200	-47.568	-4.191	0.204
4600	9.803	78.191	69.674	39.179	-48.115	3.225	0.153
4700	9.849	78.404	69.859	[illegible]0.161	-48.697	-2.250	0.105
4800	9.896	78.613	70.040	41.149	-49.308	-1.257	0.057
4900	9.944	78.818	70.218	42.141	-49.952	-0.256	0.011
5000	9.993	79.[illegible]1	70.393	43.138	-50.628	0.760	-0.033
5100	10.042	79.220	70.566	44.140	-51.336	1.789	-0.077
5200	10.092	79.417	70.735	45.147	-52.074	2.833	-0.119
5300	10.142	79.611	70.902	46.159	-52.845	3.887	-0.160
5400	10.193	79.803	71.067	47.176	-53.648	4.958	-0.201
5500	10.244	79.992	71.229	48.198	-54.483	6.044	-0.240
5600	10.296	80.178	71.388	49.22[illegible]	-55.350	7.148	-0.279
5700	10.348	80.363	71.546	50.258	-56.252	8.261	-0.317
5800	10.400	80.545	71.701	51.296	-57.190	9.398	-0.354
5900	10.453	80.725	71.854	52.339	-58.164	10.547	-0.391
6000	10.505	80.903	72.0[illegible]	[illegible]3.[illegible]	-59.179	11.714	-0.427

15 December 1962 — RCF

CALCIUM OXIDE (CaO) (IDEAL MOLECULAR GAS) gfw = 56.08

ΔH^o_{f0} = 1.095 kcal gfw-1

$\Delta H^o_{f298.15}$ = 0.800 kcal gfw^{-1}

Ground State Configuration = $^3\Sigma$

$S^o_{298.15}$ = 54.217 cal deg K^{-1}gfw^{-1}

$H^o_{298.15}-H^o_0$ = 2.117 kcal gfw-1

		cm^{-1}							
State	g	E	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e x10^5$	$D_e x10^6$
$X^3\Sigma$	-	0	850.0	5.0	-	0.53	0.004	-	0.7
$X'^1\Sigma$	-	15000	732.11	4.81	-	0.44447	0.00335	-	0.656
$^3\Sigma$	-	20000	725.0	4.0	-	0.45	0.003	-	0.7

Heat of Formation

Average heat of dissociation of 100 kcal gfw^{-1} adopted. Based on works of Brewer,[1,2] Gaydon,[3] and Ackermann et al.[4]

Heat Capacity and Entropy

Calculated on diatomic-gas program using above spectroscopic constants.

References

1. Brewer, L., Chem. Revs. 52, 1 (1953).
2. Brewer, L., U.S. AEC Rept., UCRL-8356 (1958).
3. Gaydon, A. G., Dissociation Energies, 2nd ed., Chapman and Hall, London (1953).
4. Ackermann, R. J., R. J. Thorn, and G. H. Winslow, Planet. Space Sci. 3, 12 (1961).

TABLE 130

CERIUM REFERENCE STATE **Ce**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p Solid Ce from 0° to 1077°K, Liquid from 1077° to 4271°K, Gas from 4271° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.133			
298.15	6.440	17.640	17.640	0.000			
300	6.446	17.680	17.640	0.012			
400	6.759	19.576	17.897	0.672			
500	7.096	21.120	18.391	1.364			
600	7.456	22.446	18.959	2.092			
700	7.840	23.623	19.543	2.856			
800	8.248	24.697	20.121	3.661			
900	8.680	25.695	20.685	4.507			
1000	9.135	26.631	21.235	5.397			
1003	9.149	26.658	21.250	5.425			
1003	9.047	27.356	21.250	6.125			
1077	9.047	28.000	21.692	6.794			
1077	9.345	29.449	21.692	8.032			
1100	9.345	29.647	21.850	8.247			
1200	9.345	30.160	22.509	9.182			
1300	9.345	30.908	23.126	10.116			
1400	9.345	31.601	23.707	11.051			
1500	9.345	32.245	24.255	11.985			
1600	9.345	32.849	24.774	12.920			
1700	9.345	33.415	25.266	13.854			
1800	9.345	33.949	25.733	14.789			
1900	9.345	34.454	26.179	15.723			
2000	9.345	34.934	26.605	16.658			
2100	9.345	35.390	27.013	17.592			
2200	9.345	35.825	27.403	18.527			
2300	9.345	36.240	27.779	19.461			
2400	9.345	36.648	28.139	20.396			
2500	9.345	37.014	28.487	21.330			
2600	9.345	37.386	28.822	22.265			
2700	9.345	37.736	29.146	23.199			
2800	9.345	38.078	29.459	24.134			
2900	9.345	38.406	29.762	25.068			
3000	9.345	38.723	30.055	26.003			
3100	9.345	39.029	30.340	26.937			
3200	9.345	39.326	30.616	27.872			
3300	9.345	39.614	30.884	28.806			
3400	9.345	39.893	31.145	29.741			
3500	9.345	40.163	31.399	30.675			
3600	9.345	40.427	31.646	31.610			
3700	9.345	40.683	31.887	32.544			
3800	9.345	40.932	32.122	33.479			
3900	9.345	41.175	32.351	34.413			
4000	9.345	41.411	32.574	35.348			
4100	9.345	42.023	32.793	36.282			
4200	9.345	41.642	33.006	37.217			
4270.73	9.345	41.867	33.154	37.880			
4270.73	8.202	62.396	33.154	124.889			
4300	8.216	62.452	33.352	125.127			
4400	8.264	62.641	34.016	125.951			
4500	8.312	62.826	34.655	126.780			
4600	8.360	63.011	35.269	127.614			
4700	8.407	63.191	35.860	128.452			
4800	8.453	63.369	36.433	129.295			
4900	8.498	63.543	36.984	130.142			
5000	8.542	63.715	37.516	130.994			
5100	8.584	63.885	38.032	131.851			
5200	8.624	64.052	38.531	132.711			
5300	8.663	64.217	39.014	133.576			
5400	8.699	64.379	39.482	134.444			
5500	8.734	64.539	39.936	135.315			
5600	8.766	64.697	40.377	136.190			
5700	8.795	64.852	40.805	137.068			
5800	8.822	65.005	41.221	137.949			
5900	8.846	65.156	41.625	138.833			
6000	8.868	65.305	42.019	139.718			

15 December 1962 RCF

0^oK to 1077^oK	Crystal
1077^oK to 4271^oK	Liquid
4271^oK to 6000^oK	Ideal Monatomic Gas

$\Delta H^o_{f0} = 0$ $\Delta H^o_{f298.15}$ 0

$\Delta H^o_{s298.15} = 95.000$ kcal gfw^{-1} $S^o_{298.15} = 17.640$ cal deg K^{-1}gfw^{-1}

$T_t = 1003^oK$ $\Delta H_t = 0.700$ kcal gfw^{-1}

$T_m = 1077^oK$ $\Delta H_m = 1.238$ kcal gfw^{-1}

$T_b = 4271^oK$ $\Delta H_v = 87.009$ kcal gfw^{-1}

$H^o_{298.15} - H^o_0 = 1.509$ kcal gfw^{-1}

$C^o_p = 5.649 + 2.300 \times 10^{-3}T + 11.862 \times 10^{-7}T^2$ cal deg K^{-1}gfw^{-1}

$298.15^oK \leq T \leq 1003^oK$

$C^o_p = 9.047$ cal deg K^{-1}gfw^{-1} $1003^oK \leq T \leq 1077^oK$

$C^o_p = 9.345$ cal deg K^{-1}gfw^{-1} $1077^oK \leq T \leq 4271^oK$

Structure

γ-Ce is f.c.c. from 260° to 1003°K. δ-Ce is b.c.c. from 1003° to 1077°K.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Low-temperature data estimated See volume 1, this study (section IVA5) for details. High-temperature data by Spedding et al.[1]

Melting and Vaporization

Heats of transition and fusion from Spedding et al.[1] Heat of vaporization value recommended by Spedding and Daane.[2]

References

1. Spedding, F. H. et al, J. Phys. Chem. 64, 289 (1960)
2. Spedding, F. H and A. H. Daane, Met. Rev. 5, 297 (1960).

CERIUM (Ce) (REFERENCE STATE) GFW = 140.13

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T	$-(F^o_T - H^o_{298})/T$	$H^o_T - H^o_{298}$ (Kcal gfw)	ΔH_f	ΔF_f	log K_p
298.15	±0.050	±0.800	±0.800	±0.000			
1003	±0.050	±0.830	±0.810	±0.020			
1003	±0.050	±0.838	±0.810	±0.028			
1077	±0.050	±0.840	±0.810	±0.030			
1077	±0.050	±0.844	±0.810	±0.034			
2000	±0.100	±0.900	±0.840	±0.110			
3000	±1.000	±1.120	±0.900	±0.660			
4000	±2.900	±1.680	±1.030	±2.610			
4270.73	±3.400	±1.890	±1.080	±3.460			
4270.73	±0.300	±0.770	±0.660	±0.490			
5000	±0.400	±0.830	±0.680	±0.750			
6000	±0.500	±0.910	±0.710	±1.200			

CERIUM **IDEAL MONATOMIC GAS** **Ce**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p Solid Ce from 0° to 1077°K, Liquid Ce from 1077° to 4271°K, Gaseous Ce from 4271° to 6000°K.

T, °K	C_p° (cal/°K gfw.)	S_T° (cal/°K gfw.)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw.)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw.)	ΔH_f° (Kcal/gfw.)	ΔF_f° (Kcal/gfw.)	Log K_p
0	0.000	0.000	INFINITE	-1.509	95.624	95.624	INFINITE
298.15	5.438	43.591	43.591	0.000	95.000	87.263	-63.962
300	5.447	43.625	43.591	0.010	94.998	87.215	-63.533
400	5.894	45.255	43.810	0.577	94.905	84.635	-46.240
500	6.219	46.608	44.238	1.185	94.821	82.076	-35.874
600	6.455	47.763	44.732	1.819	94.727	79.536	-28.970
700	6.666	48.774	45.239	2.475	94.619	77.013	-24.043
800	6.874	49.678	45.738	3.157	94.491	74.506	-20.353
900	7.073	50.449	46.222	3.849	94.342	72.017	-17.487
1000	7.248	51.254	46.688	4.566	94.169	69.545	-15.198
1003	7.253	51.275	46.702	4.588	94.163	69.472	-15.137
1003	7.253	51.275	46.702	4.588	93.463	69.472	-15.137
1077	7.361	51.796	47.034	5.128	93.334	67.707	-13.739
1077	7.361	51.796	47.034	5.128	92.096	67.707	-13.739
1100	7.391	51.952	47.135	5.298	92.051	67.186	-13.348
1200	7.497	51.559	47.564	6.043	91.861	64.934	-11.826
1300	7.571	53.202	47.975	6.796	91.[illegible]	62.696	-10.540
1400	7.618	53.766	48.368	7.556	91.505	60.475	-9.440
1500	7.645	54.292	48.741	8.319	91.334	58.264	-8.489
1600	7.657	54.786	49.108	9.084	91.164	56.066	-7.658
1700	7.660	55.250	49.456	9.850	90.996	53.877	-6.926
1800	7.658	55.668	49.790	10.616	90.827	51.697	-6.277
1900	7.653	56.102	50.112	11.382	90.659	49.527	-5.697
2000	7.648	56.494	50.421	12.147	90.489	47.368	-5.176
2100	7.644	56.867	50.719	12.911	90.319	45.217	-4.706
2200	7.641	57.223	51.007	13.676	90.149	43.071	-4.279
2300	7.640	57.563	51.284	14.440	89.979	40.938	-3.890
2400	7.642	57.888	51.553	15.204	89.808	38.806	-3.534
2500	7.647	58.200	51.813	15.968	89.638	36.685	-3.207
2600	7.655	58.500	52.064	16.733	89.468	34.571	-2.906
2700	7.666	58.789	52.308	17.499	89.300	32.463	-2.628
2800	7.680	59.066	52.544	18.267	89.133	30.367	-2.370
2900	7.698	59.338	52.774	19.036	88.968	28.265	-2.130
3000	7.718	59.599	52.99[illegible]	19.806	88.803	26.174	-1.907
3100	7.742	59.853	53.214	20.579	88.[illegible]	24.091	-1.698
3200	7.769	60.099	53.425	21.355	88.48	22.011	-1.503
3300	7.799	60.338	53.631	22.133	88.327	19.935	-1.320
3400	7.832	60.572	53.832	22.915	88.174	17.864	-1.148
3500	7.867	60.799	54.028	23.700	88.02[illegible]	15.798	-0.986
3600	7.905	61.021	54.219	24.488	87.878	13.737	-0.834
3700	7.945	61.239	54.406	25.281	87.737	11.680	-0.690
3800	7.987	61.451	54.568	26.077	87.598	9.629	-0.554
3900	8.030	61.659	54.767	26.878	87.465	7.578	-0.425
4000	8.075	61.863	54.94[illegible]	27.683	87.335	5.528	-0.302
4100	8.122	62.063	55.113	28.493	87.211	3.488	-0.186
4200	8.167	62.259	55.281	29.308	87.091	1.445	-0.075
4270.73	8.202	62.396	55.398	29.889	87.009	0.000	0.000
4270.73	8.202	62.396	55.398	29.889			
4300	8.216	62.452	55.446	30.127			
4400	8.264	62.641	55.607	30.951			
4500	8.312	62.828	55.765	31.780			
4600	8.360	63.011	55.921	.614			
4700	8.407	63.191	56.074	33.452			
4800	8.453	63.369	56.224	34.295			
4900	8.498	63.543	56.371	35.142			
5000	8.542	63.715	56.517	35.994			
5100	8.584	63.885	56.659	36.851			
5200	8.624	64.052	56.800	37.711			
5300	8.663	64.217	56.938	38.576			
5400	8.699	64.379	57.071	39.444			
5500	8.734	64.539	57.203	40.315			
5600	8.766	64.697	57.341	41.190			
5700	8.796	64.852	57.47[illegible]	42.068			
5800	8.822	65.005	57.602	42.949			
5900	8.846	65.156	57.72[illegible]	43.833			
6000	8.868	65.305	57.8[illegible]	44.718			

15 December 1962 RCF

CERIUM (Ce) (IDEAL MONATOMIC GAS) gfw = 140.13

ΔH^o_{f0} = 95.624 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 95.000 kcal gfw^{-1}

Ground State Configuration = $^2D_{1\frac{1}{2}}$

$S^o_{298.15}$ = 43.591 cal deg K^{-1}gfw^{-1}

$H^o_{298.15}-H^o_0$ = 1.509 kcal gfw^{-1}

Electronic Levels and Multiplicities

Electronic levels for Ce were assumed to be same as those for La as given by Moore.[1]

Heat of Formation

Based on several values. Value by Spedding and Daane[2] adopted.

Heat Capacity and Entropy

Calculated on monatomic-gas computer program.

References

1. Moore, C., Atomic Energy Levels, Vol. 3, Nat. Bur. Stds. (U.S.) (1958).
2. Spedding, F. H. and A. H. Daane, Met. Rev. 5, 297 (1960).

CERIUM, MONATOMIC (Ce) (IDEAL GAS) GFW = 140.13

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw			Kcal/gfw			log K_p
	C^o_p	S^o_T	$-(F^o_T - H^o_{298})/T$	$H^o_T - H^o_{298}$	ΔH_f	ΔF_f	
298.15	± 0.200	±0.500	±0.500	±0.000	± 2.500	± 2.890	± 2.120
1003	± 0.150	±0.590	±0.540	±0.050	± 2.570	± 3.850	± 0.840
1003	± 0.150	±0.590	±0.540	±0.050	± 2.580	± 3.850	± 0.840
1077	± 0.150	±0.600	±0.540	±0.060	± 2.590	± 3.950	± 0.800
1077	± 0.150	±0.600	±0.540	±0.060	± 2.600	± 3.950	± 0.800
2000	± 0.100	±0.670	±0.590	±0.170	± 2.780	± 5.360	± 0.590
3000	± 0.100	±0.710	±0.620	±0.270	± 3.430	± 7.060	± 0.510
4000	± 0.200	±0.760	±0.650	±0.420	± 5.530	± 9.220	± 0.500
4270.73	± 0.300	±0.770	±0.660	±0.490	± 6.450	± 9.930	± 0.510
4270.73	± 0.300	±0.770	±0.660	±0.490			
5000	± 0.400	±0.830	±0.680	±0.750			
6000	± 0.500	±0.910	±0.710	±1.200			

CERIUM OXIDE

IDEAL MOLECULAR GAS

CeO

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ce from 0° to 1077°K, Liquid Ce from 1077° to 4271°K, Gaseous Ce from 4271° to 6000°K, Gaseous O_2, Gaseous CeO.

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-2.114	-30.044	-30.044	INFINITE
298.15	7.521	57.219	57.219	0.000	-31.100	-35.595	26.090
300	7.529	57.266	57.200	0.014	-31.105	-35.617	25.946
400	7.915	59.487	57.520	0.787	-31.347	-37.092	20.265
500	8.196	61.285	58.099	1.593	-31.598	-38.501	16.828
600	8.391	62.798	58.759	2.423	-31.874	-39.855	14.516
700	8.528	64.103	59.432	3.270	-32.180	-41.162	12.851
800	8.626	65.248	60.088	4.128	-32.526	-42.421	11.588
900	8.699	66.269	60.719	4.994	-32.913	-43.636	10.596
1000	8.755	67.188	61.321	5.867	-33.344	-44.805	9.792
1003	8.756	67.213	61.338	5.893	-33.358	-44.838	9.769
1003	8.756	67.213	61.338	5.893	-34.058	-44.838	9.769
1077	8.789	67.837	61.763	6.543	-34.387	-45.621	9.257
1077	8.789	67.837	61.763	6.543	-35.625	-45.621	9.257
1100	8.799	68.025	61.893	6.745	-35.735	-45.834	9.106
1200	8.834	68.792	62.436	7.626	-36.213	-46.731	8.510
1300	8.864	69.500	62.953	8.511	-36.[illegible]71	-47.590	8.000
1400	8.889	70.158	63.444	9.399	-37.170	-48.410	7.557
1500	8.911	70.772	63.913	10.289	-37.649	-49.197	7.168
1600	8.933	71.348	64.360	11.181	-38.130	-49.950	6.823
1700	8.954	71.890	64.787	12.076	-38.611	-50.674	6.514
1800	8.975	72.402	65.196	12.972	-39.094	-51.371	6.237
1900	8.999	72.888	65.588	13.871	-39.576	-52.039	5.986
2000	9.025	73.351	65.965	14.772	-40.060	-52.682	5.757
2100	9.054	73.792	66.327	15.676	-40.543	-53.300	5.547
2200	9.087	74.214	66.676	16.583	-41.027	-53.897	5.354
2300	9.125	74.618	67.013	17.493	-41.509	-54.471	5.176
2400	9.167	75.008	67.338	18.408	-41.990	-55.027	5.011
2500	9.215	75.383	67.652	19.327	-42.469	-55.559	4.857
2600	9.268	75.745	67.957	20.251	-42.946	-56.074	4.713
2700	9.325	76.096	68.252	21.181	-43.419	-56.570	4.579
2800	9.387	76.437	68.538	22.116	-43.889	-57.048	4.453
2900	9.454	76.767	68.816	23.058	-44.356	-57.509	4.334
3000	9.525	77.089	69.087	24.007	-44.817	-57.958	4.222
3100	9.600	77.403	69.350	24.963	-45.[illegible]	-58.385	4.116
3200	9.678	77.709	69.607	25.927	-45.7[illegible]	-58.804	4.016
3300	9.759	78.008	69.857	26.899	-46.17	-59.206	3.921
3400	9.842	78.301	70.101	27.879	-46.610	-59.594	3.830
3500	9.926	78.588	70.340	28.868	-47.043	-59.970	3.745
3600	10.012	78.[illegible]69	70.573	29.864	-47.471	-60.334	3.663
3700	10.098	79.144	70.801	30.870	-47.889	-60.685	3.584
3800	10.184	79.415	71.024	31.884	-48.303	-61.023	3.509
3900	10.270	79.681	71.243	32.907	-48.708	-61.354	3.438
4000	10.355	79.942	71.458	33.938	-49.108	-61.678	3.370
4100	10.439	80.199	71.668	34.978	-49.500	-61.985	3.304
4200	10.521	80.452	71.874	36.026	-49.857	-62.285	3.241
4270.73	10.578	80.629	72.018	36.775	-50.157	-62.494	3.198
4270.73	10.578	80.629	72.018	36.775	-137.166	-62.494	3.198
4300	10.601	80.701	72.077	37.082	-137.243	-61.987	3.150
4400	10.679	80.945	72.276	38.146	-1[illegible].507	-60.232	2.992
4500	10.754	81.187	72.472	39.217	-137.770	-58.474	2.840
4600	10.827	81.474	72.664	40.296	-138.033	-56.708	2.694
4700	10.896	81.658	72.853	41.382	-138.296	-54.943	2.555
4800	10.963	81.888	73.039	42.475	-138.559	-53.158	2.420
4900	11.026	82.115	73.223	43.575	-138.823	-51.384	2.292
5000	11.087	82.339	73.403	44.680	-139.090	-49.600	2.168
5100	11.144	82.560	73.581	45.792	-139.360	-47.808	2.049
5200	11.197	82.777	73.756	46.909	-139.633	-46.008	1.934
5300	11.247	82.991	73.929	48.031	-139.913	-44.210	1.823
5400	11.295	83.202	74.099	49.158	-140.198	-42.402	1.716
5500	11.338	83.410	74.267	50.289	-140.490	-40.590	1.613
5600	11.379	83.616	74.432	51.425	-140.792	-38.769	1.513
5700	11.417	83.818	74.596	52.565	-141.107	-36.948	1.417
5800	11.451	84.017	74.757	53.708	-141.437	-35.116	1.323
5900	11.483	84.214	74.916	54.854	-141.785	-33.283	1.233
6000	11.512	84.407	75.07[illegible]	56.004	-142.153	-31.436	1.145

15 December 1962 RCF

CERIUM MONOXIDE (CeO) (IDEAL MOLECULAR GAS) gfw = 156.13

ΔH^o_{f0} = - 30 044 kcal gfw^{-1}

Ground State Degeneracy = 2

$H^o_{298.15} - H^o_0$ = 2 114 kcal gfw^{-1}

$\Delta H^o_{f298\ 15}$ = - 31.1 kcal gfw^{-1}

$S^o_{298.15}$ = 57 219 cal deg K^{-1} gfw^{-1}

State	g	E (cm^{-1})	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e \times 10^5$	$D_e \times 10^6$
X	2	0	865	2.99	—	0.359	—	—	0 25
A	2	12764 3	785.3	2.13	—	0.326	—	—	0.22
B	2	13817 2	788.3	1 76	—	0.327	—	—	0.23
X'	2	13720.	840.2	2 58	—	0 349	—	—	0.23
D	2	34276.	791.7	1.72	—	0.329	—	—	0 23
E	2	34584	807 9	2.04	—	0.335	—	—	0 23

Heat of Formation

Based on data of Walsh, Dever, and White.[1] See volume 1, this study (section IVB5. 4) for details.

Heat Capacity and Entropy

Calculated using above spectroscopic constants, which are from Herzberg[2] or have been estimated.

References

1. Walsh, P. N., D F. Dever, and D White, J Phys. Chem 65, 1410 (1961).
2. Herzberg, G , Spectra of Diatomic Molecules I., 2nd ed, Van Nostrand, N. Y (1950)

CHROMIUM

REFERENCE STATE

Cr

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p. Solid Cr from 0° to 2148°K, Liquid Cr from 2148 to 2967°K, Gaseous Cr from 2967 to 6000°K.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-0.970			
298.15	5.577	5.680	5.680	0.000			
300	5.579	5.714	5.681	0.010			
311.65	5.597	5.934	5.687	0.077			
311.65	5.597	5.938	5.687	0.078			
400	5.800	7.400	5.913	0.595			
500	6.090	8.794	6.354	1.220			
600	6.415	9.978	6.861	1.870			
700	6.755	10.995	7.380	2.530			
800	7.103	11.902	7.890	3.210			
900	7.455	12.726	8.382	3.910			
1000	7.810	13.495	8.855	4.640			
1100	8.167	14.229	9.310	5.410			
1200	8.525	14.942	9.750	6.230			
1300	8.884	15.638	10.177	7.100			
1400	9.243	16.312	10.591	8.010			
1500	9.603	16.961	10.994	8.950			
1600	9.964	17.587	11.387	9.920			
1648	10.137	17.882	11.571	10.400			
1648	10.137	18.368	11.571	11.200			
1700	10.324	18.684	11.784	11.730			
1800	10.685	19.284	12.184	12.780			
1900	11.046	19.879	12.573	13.880			
2000	11.408	20.463	12.953	15.020			
2088	11.726	20.975	13.281	16.065			
2088	11.726	21.142	13.281	16.415			
2100	11.769	21.212	13.327	16.560			
2148	11.942	21.486	13.517	17.117			
2148	9.400	23.786	13.517	2.057			
2200	9.400	24.[illegible]1	13.763	22.545			
2300	9.400	24.479	14.218	23.485			
2400	9.400	24.829	14.652	24.425			
2500	9.400	25.213	15.067	25.365			
2600	9.400	25.581	15.464	26.305			
2700	9.400	25.936	15.845	27.245			
2800	9.400	26.278	16.212	28.185			
2900	9.400	26.608	16.565	29.125			
2967	9.400	26.822	16.794	29.755			
2967	7.317	53.861	16.794	109.974			
3000	7.352	53.943	17.204	110.216			
3100	7.481	54.186	18.393	110.958			
3200	7.599	54.425	19.515	111.712			
3300	7.713	74.661	20.577	112.478			
3400	7.825	54.893	21.583	113.255			
3500	7.935	55.121	22.537	114.043			
3600	8.045	55.346	23.445	114.842			
3700	8.157	55.568	24.311	115.652			
3800	8.270	55.787	25.136	116.473			
3900	8.386	56.004	25.926	117.306			
4000	8.506	56.217	26.679	118.151			
4100	8.631	56.429	27.402	119.008			
4200	8.761	56.638	28.096	119.877			
4300	8.896	56.846	28.762	120.760			
4400	9.036	57.052	29.403	21.657			
4500	9.183	57.257	30.020	122.567			
4600	9.335	57.460	30.614	123.493			
4700	9.492	57.663	31.187	124.435			
4800	9.654	57.864	31.741	125.392			
4900	9.821	58.065	32.276	126.366			
5000	9.992	58.265	32.794	127.356			
5100	10.167	58.465	33.296	128.364			
5200	10.344	58.664	33.781	129.390			
5300	10.524	58.863	34.253	130.433			
5400	10.705	59.061	34.710	131.495			
5500	10.887	59.259	35.155	132.574			
5600	11.069	59.457	35.587	133.672			
5700	11.250	59.[illegible]5	36.008	134.788			
5800	11.429	59.852	36.417	135.922			
5900	11.605	60.049	36.816	137.074			
6000	11.779	60.245	37.204	138.243			

May 1962

CHW

CHROMIUM (Cr) (REFERENCE STATE) gfw = 52.01

$0^{o}K$ to $2148^{o}K$ Crystal

$2148^{o}K$ to 2967^{o} K Liquid

$2967^{o}K$ to $6000^{o}K$ Ideal Monatomic Gas

$\Delta H^{o}_{f0} = 0$

$\Delta H^{o}_{f298.15} = 0$

$\Delta H^{o}_{s298.15} = 94.820$ kcal gfw^{-1}

$S^{o}_{298.15} = 5.68$ cal $degK^{-1}$ gfw^{-1}

$T_t = 311.65^{o}K$

$\Delta H_t = 0.0014$ kcal gfw^{-1}

$T_t = 1648^{o}K$

$\Delta H_t = 0.800$ kcal gfw^{-1}

$T_t = 2088^{o}K$

$\Delta H_t = 0.350$ kcal gfw^{-1}

$T_m = 2148^{o}K$

$\Delta H_m = 4.92$ kcal gfw^{-1}

$T_b = 2967^{o}K$

$\Delta H_v = 80.220$ kcal gfw^{-1}

$H^{o}_{298.15} - H^{o}_{0} = 0.970$ kcal gfw^{-1}

Structure

The stable form at $298.15^{o}K$ is b. c. c., an antiferromagnetic transition occurs at $311.65^{o}K$. A second occurs at $1648^{o}K$. At $2088^{o}K$, the b. c. c. transforms into f. c. c. structure.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Low-temperature data from earlier works of Hultgren and identical with their final tabulation.[1] High-temperature data primarily from Kelley.[2] Data for liquid estimated.

Melting

An average of five determinations used.

Vaporization

An average of five determinations used.

Further details by Barriault et al.[3]

References

1. Hultgren, R. et al, Selected Values of Thermodynamic Properties of Metals and Alloys, Wiley, New York (1963).
2. Kelley, K., U. S. Bur. Mines, Bull. 584 (1960).
3. Barriault, R. J. et al, ASD TR 61-260 (May 1962), Pt. 1.

CHROMIUM (Cr) (REFERENCE STATE) GFW = 52.01

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw C^{o}_{p}	S^{o}_{T}	$-(F^{o}_{T} - H^{o}_{298})/T$	Kcal/gfw $H^{o}_{T} - H^{o}_{298}$	ΔH^{o}_{f}	ΔF^{o}_{f}	Log K_p
298.15	±0.200	±0.070	±0.070	±0.000			
311.65	±0.200	±0.080	±0.070	±0.003			
311.65	±0.200	±0.080	±0.070	±0.003			
1000	±0.700	±0.600	±0.290	±0.310			
1648	±1.200	±1.070	±0.510	±0.930			
1648	±1.200	±1.190	±0.510	±1.130			
2000	±1.200	±1.420	±0.640	±1.550			
2088	±1.200	±1.470	±0.680	±1.660			
2088	±1.200	±1.520	±0.680	±1.760			
2184	±1.200	±1.550	±0.700	±1.830			
2184	±1.000	±2.020	±0.700	±2.830			
2967	±1.000	±2.340	±1.450	±2.650			
2967	±0.000	±0.003					
3000	±0.001						
4000	±0.001	±0.003					
5000	±0.002	±0.003					
6000	±0.002	±0.003					

TABLE 134

CHROMIUM — IDEAL MONATOMIC GAS — **Cr**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Cr from 0° to 2148°K, Liquid Cr from 2148° to 2967°K, Gaseous Cr from 2967° to 6000°K.

T, °K	cal/°K gfw C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	Kcal/gfw $H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.481	94.309	94.309	INFINITE
298.15	4.968	41.637	41.637	0.000	94.820	84.099	-61.644
300	4.968	41.668	41.637	0.009	94.819	84.033	-61.215
311.65	4.968	41.857	41.642	0.067	94.810	83.615	-58.633
311.65	4.968	41.857	41.642	0.067	94.809	83.615	-58.633
400	4.968	43.097	41.832	0.506	94.731	80.452	-43.955
500	4.968	44.206	42.200	1.003	94.603	76.897	-33.610
600	4.968	45.111	42.612	1.500	94.450	73.369	-26.723
700	4.968	45.877	43.025	1.996	94.286	69.868	-21.813
800	4.969	46.541	43.424	2.493	94.103	66.393	-18.137
900	4.972	47.126	43.803	2.990	93.900	62.942	-15.284
1000	4.980	47.650	44.162	3.488	93.668	59.513	-13.006
1100	4.996	48.126	44.501	3.987	93.397	56.109	-11.147
1200	5.023	48.561	44.822	4.487	93.077	52.734	-9.604
1300	5.065	48.965	45.125	4.992	92.712	49.387	-8.302
1400	5.125	49.342	45.413	5.501	92.311	46.070	-7.191
1500	5.203	49.698	45.687	6.017	91.887	42.780	-6.233
1600	5.300	50.037	45.948	6.542	91.442	39.523	-5.398
1648	5.353	50.195	46.070	6.798	91.218	37.965	-5.034
1648	5.353	50.195	46.070	6.798	90.418	37.965	-5.034
1700	5.414	50.362	46.199	7.078	90.168	36.314	-4.668
1800	5.545	50.675	46.439	7.626	89.666	33.161	-4.026
1900	5.688	50.979	46.670	8.187	89.127	30.035	-3.455
2000	5.841	51.274	46.892	8.763	88.563	26.222	-2.865
2088	5.982	51.529	47.082	9.284	88.039	24.244	-2.537
2088	5.982	51.529	47.082	9.284	87.689	24.244	-2.537
2100	6.001	51.563	47.108	9.356	87.616	23.879	-2.485
2148	6.080	51.700	47.209	9.646	87.349	22.449	-2.284
2148	6.080	51.700	47.209	.646	82.409	22.449	-2.284
2200	6.165	51.846	47.317	9.964	82.239	21.001	-2.086
2300	6.330	52.124	47.520	10.589	81.924	18.225	-1.732
2400	6.493	52.397	47.717	11.230	81.625	15.463	-1.408
2500	6.652	52.665	47.910	11.887	81.342	12.713	-1.111
2600	6.806	52.929	48.098	12.560	81.075	9.971	-0.838
2700	6.954	53.188	48.282	13.248	80.823	7.241	-0.586
2800	7.095	53.444	48.462	13.951	80.586	4.519	-0.353
2900	7.240	53.695	48.638	14.667	80 [illegible]	1.810	-0.136
2967	7.317	53.8[illegible]1	48.754	15.154	80.2[illegible]	0.000	0.000
2967	7.317	53.861	48.754	15.154			
3000	7.359	53.943	48.810	15.396			
3100	7.481	54.186	48.980	16.138			
3200	7.599	54.425	49.146	16.892			
3300	7.713	54.661	49.310	17.658			
3400	7.825	54.893	49.471	18.435			
3500	7.935	55.121	49.629	19.223			
3600	8.045	55.346	49.785	20.022			
3700	8.157	55.568	49.938	20.832			
3800	8.270	55.787	50.089	21.653			
3900	8.386	56.004	50.238	22.486			
4000	8.506	56.217	50.385	23.331			
4100	8.641	56.429	50.529	24.188			
4200	8.761	56.638	50.672	25.057			
4300	8.896	56.846	50.814	25.940			
4400	9.036	57.052	50.953	26.837			
4500	9.183	57.257	51.091	27.747			
4600	9.335	57.460	51.227	28.673			
4700	9.492	57.663	51.362	29.615			
4800	9.654	57.864	51.495	30.572			
4900	9.821	58.065	51.627	31.546			
5000	9.992	58.265	51.758	32.536			
5100	10.167	58.465	51.888	33.544			
5200	10.344	58.664	52.016	34.570			
5300	10.524	58.863	52.143	35.613			
5400	10.705	59.061	52.270	36.675			
5500	10.887	59.259	52.395	37.754			
5600	11.069	59.457	52.519	38.852			
5700	11.250	59.655	52.643	39.968			
5800	11.429	59.852	52.765	41.102			
5900	11.605	60.049	52.887	42.254			
6000	11.779	60.245	53.008	43.423			

May 1962 — CHW

CHROMIUM (Cr) (IDEAL MONATOMIC GAS) gfw = 52.01

ΔH^o_{f0} = 94.309 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 94.820 kcal gfw^{-1}

Ground State Configuration = $^7S_3$

$S^o_{298.15}$ = 41.637 cal $degK^{-1}$ gfw^{-1}

$H^o_{298.15} - H^o_0$ = 1.481 kcal gfw^{-1}

Electronic Levels and Multiplicities

Energy levels from Moore.[1]

Heat of Formation

Vapor-pressure measurements from five sources used.

Heat Capacity and Entropy

Calculated using monatomic-gas program.

Further details by Barriault et al.[2]

References

1. Moore, C. Atomic Energy Levels, Vol. 2, Nat. Bur. Stds. (1952).
2. Barriault, R. et al, ASD TR 61-260 (May 1962), Pt. I.

CHROMIUM, MONATOMIC (Cr) (IDEAL GAS) GFW = 52.01

SUMMARY OF UNCERTAINTY ESTIMATES

T °K	C_p^o (cal/°K gfw)	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$ (kcal/gfw)	ΔH_f^o	ΔF_f^o	Log K_p
298.15	±0.000	±0.002	±0.002	±0.000	±0.500	±0.520	±0.380
311.65	±0.000	±0.002	±0.002	±0.000	±0.500	±0.520	±0.360
311.65	±0.000	±0.002	±0.002	±0.000	±0.500	±0.520	±0.360
1000	±0.000	±0.002	±0.002	±0.000	±0.810	±0.790	±0.170
1648	±0.000	±0.002	±0.002	±0.000	±1.430	±1.340	±0.180
1648	±0.000	±0.002	±0.002	±0.000	±1.630	±1.340	±0.180
2000	±0.001	±0.002	±0.003	±0.000	±2.050	±1.790	±0.200
2088	±0.001	±0.002	±0.003	±0.000	±2.160	±1.930	±0.200
2088	±0.001	±0.002	±0.003	±0.000	±2.260	±1.930	±0.200
2148	±0.001	±0.002	±0.003	±0.001	±2.330	±2.010	±0.200
2148	±0.001	±0.002	±0.003	±0.001	±3.330	±2.010	±0.200
2967	±0.001	±0.003	±0.003	±0.001	±3.150	±4.810	±0.350
2967	±0.001	±0.003	±0.003	±0.001			
3000	±0.001	±0.003	±0.003	±0.001			
4000	±0.001	±0.003	±0.003	±0.002			
5000	±0.002	±0.003	±0.003	±0.003			
6000	±0.002	±0.003	±0.003	±0.005			

TABLE 135

CHROMIUM MONOXIDE — IDEAL MOLECULAR GAS — CrO

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Cr from 0° to 2148°K, Liquid Cr from 2148° to 2967°K, Gaseous Cr from 2967° to 6000°K, Gaseous O_2, Gaseous CrO.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.440	49.567	49.567	INFINITE
298.15	8.288	56.689	56.689	0.000	50.000	42.098	-30.857
300	8.289	56.740	56.689	0.015	49.998	42.049	-30.631
311.65	8.296	57.057	56.697	0.112	49.987	41.744	-29.272
311.65	8.296	57.057	56.697	0.112	49.986	41.744	-29.272
400	8.397	59.138	57.015	0.849	49.893	39.416	-21.535
500	8.526	61.025	57.635	1.695	49.748	36.813	-16.090
600	8.635	62.590	58.334	2.554	49.579	34.241	-12.472
700	8.720	63.928	59.040	3.421	49.397	31.699	-9.896
800	8.786	65.096	59.725	4.297	49.194	29.185	-7.973
900	8.838	66.134	60.381	5.178	48.968	26.697	-6.483
1000	8.880	67.068	61.004	6.064	48.711	24.234	-5.296
1100	8.915	67.916	61.594	6.954	48.411	21.801	-4.331
1200	8.945	68.693	62.154	7.847	48.060	19.397	-3.532
1300	8.971	69.410	62.685	8.743	47.658	17.026	-2.862
1400	8.994	70.076	63.189	9.641	47.214	14.686	-2.292
1500	9.016	70.697	63.669	10.541	46.738	12.378	-1.803
1600	9.036	71.279	64.127	11.444	46.235	10.104	-1.380
1648	9.045	71.547	64.339	11.878	45.975	9.021	-1.196
1648	9.045	71.547	64.339	11.878	45.175	9.021	-1.196
1700	9.054	71.778	64.564	12.349	44.886	7.886	-1.014
1800	9.072	72.346	64.987	13.255	44.298	5.728	-0.695
1900	9.089	72.837	65.383	14.163	43.659	3.601	-0.414
2000	9.106	73.304	65.768	15.073	42.979	1.508	-0.165
2088	9.121	73.696	66.094	15.875	42.337	-0.303	0.032
2088	9.121	73.696	66.094	15.875	41.987	-0.303	0.032
2100	9.123	73.749	66.137	15.984	41.897	-0.540	0.056
2148	9.132	73.955	66.310	16.422	41.559	-1.489	0.151
2148	9.132	73.955	66.310	16.422	36.619	-1.489	0.151
2200	9.141	74.174	66.493	16.897	36.370	-2.402	0.239
2300	9.159	74.581	66.936	17.812	35.886	-4.154	0.395
2400	9.178	74.971	67.167	18.729	35.402	-5.882	0.536
2500	9.197	75.346	67.487	19.548	34.918	-7.595	0.664
2600	9.218	75.708	67.797	20.569	34.432	-9.290	0.781
2700	9.240	76.056	68.097	21.492	33.947	-10.962	0.887
2800	9.263	76.393	68.387	22.417	33.468	-12.617	0.985
2900	9.288	76.719	68.669	[illegible].344	32.[illegible]	-14.251	1.074
2966.82	9.306	76.932	68.854	23.967	32.64	-15.345	1.130
2966.82	9.306	76.932	68.854	23.967	-47.572	-15.345	1.130
3000	9.315	77.035	68.943	24.274	-47.664	-14.976	1.091
3100	9.343	77.341	69.210	25.707	-47.771	-13.888	0.979
3200	9.373	77.635	69.469	26.143	-48.250	-12.784	0.873
3300	9.404	77.928	69.772	27.082	-48.560	-11.672	0.773
3400	9.438	78.210	69.968	28.024	-48.879	-10.550	0.678
3500	9.473	78.485	70.208	28.970	-49.208	-9.426	0.589
3600	9.510	78.753	70.442	29.919	-49.547	-8.287	0.503
3700	9.548	79.015	70.671	30.872	-49.895	-7.134	0.421
3800	9.589	79.271	70.894	31.829	-50.255	-5.977	0.344
3900	9.630	79.521	71.111	32.790	-50.618	-4.805	0.269
4000	9.674	79.766	71.328	33.755	-50.994	-3.644	0.199
4100	9.719	80.007	71.537	34.725	-51.379	-2.448	0.130
4200	9.765	80.243	71.743	35.700	-51.773	-1.256	0.065
4300	9.812	80.474	71.944	36.679	-52.179	- .052	0.003
4400	9.861	80.702	72.142	37.663	-52.595	1.162	-0.058
4500	9.911	80.925	72.336	38.652	-53.022	2.381	-0.116
4600	9.962	81.145	72.526	39.647	-53.461	3.616	-0.172
4700	10.014	81.361	72.713	40.646	-53.915	4.855	-0.226
4800	10.067	81.574	72.897	41.651	-54.380	6.101	-0.278
4900	10.120	81.784	73.077	42.662	-54.860	7.360	-0.328
5000	10.175	81.991	73.255	43.678	-55.354	8.630	-0.377
5100	10.230	82.195	73.430	44.699	-55.866	9.909	-0.425
5200	10.286	82.396	73.602	45.727	-56.394	11.196	-0.471
5300	10.343	82.595	73.772	46.760	-56.941	12.492	-0.515
5400	10.400	82.791	73.939	47.800	-57.506	13.797	-0.558
5500	10.457	82.984	74.104	48.845	-58.093	15.109	-0.600
5600	10.515	83.176	74.266	49.897	-58.702	16.442	-0.642
5700	10.574	83.365	74.426	50.954	-59.338	17.778	-0.682
5800	10.633	83.553	74.584	52.018	-59.999	19.128	-0.721
5900	10.692	83.738	74.740	53.089	-60.691	20.485	-0.759
6000	10.751	83.921	74.894	54.165	-61.418	21.852	-0.796

15 September 1962 — CHW

CHROMIUM MONOXIDE (CrO) (IDEAL MOLECULAR GAS) gfw = 68.01

ΔH_{f0} = 49.567 Kcal gfw^{-1} $\Delta H^{\circ}_{f298.15}$ = 50.000 Kcal gfw^{-1}

Ground State Configuration $^{1}\Sigma$ $S^{\circ}_{298.15}$ = 56.689 cal deg K^{-1} gfw^{-1}

$H^{\circ}_{298.15}-H^{\circ}_{0}$ = 2.440 Kcal gfw^{-1}

Spectroscopic constants for ten electronic levels from Herzberg[1] were used. See text for details.

Heat of Formation

Based on work of Grimley *et al*[2].

Heat and Capacity and Entropy

Calculated on diatomic gas computer program.

References

1. Herzberg, G., Molecular Spectra and Molecular Structure I., Van Nostrand, N. Y. (1950).

2. Grimley, R., *et al.* J. Chem. Phys. 34, 664 (1961).

TABLE 136

CHROMIUM DIOXIDE — **CONDENSED PHASE** — CrO_2

Reference State for Calculating ΔH°_f, ΔF°_f, and Log Kp: Solid Cr from 0° to 2148°K, Liquid Cr from 2148° to 2967°K, Gaseous Cr from 2967 to 6000°K; Gaseous O_2; Solid CrO_2.

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal/gfw)	ΔH°_f (Kcal/gfw)	ΔF°_f (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.900	-138.855	-138.855	INFINITE
298.15	13.380	9.900	9.900	0.000	-140.000	-126.647	27.677
300	13.430	9.983	9.903	0.024	-139.999	-126.600	27.667
311.65	13.670	10.501	9.914	0.183	-139.990	-126.034	27.543
311.65	13.670	10.501	9.914	0.183	-139.991	-126.034	27.543
400	15.070	14.094	10.451	1.457	-139.861	-122.102	26.684
500	16.150	17.584	11.542	3.021	-139.653	-117.687	25.719
600	17.000	20.602	12.802	4.680	-139.400	-113.315	24.764
700	17.740	23.279	14.112	6.417	-139.100	-108.991	23.819
800	18.430	25.693	15.410	8.226	-138.769	-104.711	22.883

15 September 1962 — CHW

CHROMIUM DIOXIDE (CrO_2) (CONDENSED PHASE) gfw = 84.01

$\Delta H^\circ_{f298.15}$ = -140.000 Kcal gfw^{-1} $S^\circ_{298.15}$ = 9.900 cal deg K^{-1}gfw^{-1}

$H^\circ_{298.15}-H^\circ_0$ = 1.900 Kcal gfw^{-1}

$C^\circ_p = 14.13 + 5.80 \times 10^{-3}\ T - 2.20 \times 10^5\ T^{-2}$ cal deg K^{-1} gfw^{-1}

$298.15\ ^\circ K \leq T \leq 800\ ^\circ K$

Structure

CrO_2 is considered to remain solid until decomposition occurs near 800°K.

Heat of Formation

Based on work of Ariya *et al.*[1]

Heat Capacity and Entropy

Data were estimated.

References

1. Ariya, S., *et al.*, J. Gen. Chem. USSR 23, 1307 (1953).

TABLE 137

CHROMIUM DIOXIDE | **IDEAL MOLECULAR GAS** | **CrO_2**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Cr from 0° to 2148°K, Liquid Cr from 2148° to 2967°K, Gaseous Cr from 2967° to 6000°K, Gaseous O_2; Gaseous CrO_2.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.640	-18.595	-18.595	INFINITE
298.15	10.453	61.856	61.856	0.000	-19.000	-21.137	15.493
300	10.473	61.921	61.856	0.019	-19.004	-21.150	15.407
311.65	10.599	62.322	61.866	0.142	-19.031	-21.225	14.884
311.65	10.599	62.322	61.866	0.142	-19.032	-21.225	14.884
400	11.422	65.071	62.279	1.117	-19.201	-21.833	11.928
500	12.085	67.696	63.107	2.294	-19.380	-22.470	9.821
600	12.537	69.942	64.064	3.527	-19.553	-23.072	8.403
700	12.849	71.899	65.046	4.797	-19.720	-23.645	7.382
800	13.070	73.630	66.013	6.093	-19.902	-24.194	6.609
900	13.230	75.179	66.947	7.409	-20.100	-24.719	6.002
1000	13.350	76.580	67.842	8.738	-20.329	-25.220	5.512
1100	13.441	77.857	68.695	10.078	-20.598	-25.697	5.105
1200	13.512	79.029	69.508	11.426	-20.918	-26.146	4.762
1300	13.569	80.113	70.282	12.780	-21.291	-26.566	4.466
1400	13.614	81.120	71.021	14.139	-21.706	-26.958	4.208
1500	13.651	82.061	71.726	15.502	-22.153	-27.318	3.980
1600	13.681	82.943	72.400	16.869	-22.633	-27.646	3.776
1648	13.694	83.348	72.713	17.526	-22.880	-27.798	3.686
1648	13.694	83.348	72.713	17.526	-23.680	-27.798	3.686
1700	13.707	83.773	73.045	18.239	-23.956	-27.921	3.589
1800	13.728	84.557	73.663	19.610	-24.524	-28.138	3.416
1900	13.747	85.300	74.256	20.984	-25.144	-28.321	3.258
2000	13.762	[illegible]	74.826	22.360	-25.808	-28.470	3.111
2088	13.774	86.599	75.310	23.571	-26.439	-28.576	2.991
2088	13.774	86.599	75.310	23.571	-26.789	-28.576	2.991
2100	13.776	86.677	75.374	23.737	-26.877	-28.581	2.974
2148	13.782	86.989	75.630	24.398	-27.210	-28.594	2.909
2148	13.782	86.989	75.630	24.398	-32.150	-28.594	2.909
2200	13.788	87.319	75.903	25.115	-32.395	-28.501	2.831
2300	13.798	87.932	76.413	26.494	-32.872	-28.315	2.690
2400	13.807	88.519	76.905	27.674	-33.354	-28.106	2.559
2500	13.815	89.083	77.381	29.256	-33.840	-27.878	2.437
2600	13.822	89.625	77.841	30.637	-34.331	-27.628	2.322
2700	13.829	90.147	78.288	32.020	[illegible]	-27.365	2.215
2800	13.834	90.650	78.720	[illegible]	[illegible]	-27.076	2.113
2900	13.840	91.135	79.140	34.787	[illegible]	-26.773	2.018
2966.82	13.843	91.451	79.414	35.714	-36.170	-26.561	1.956
2966.82	13.843	91.451	79.414	35.714	-116.389	-26.561	1.956
3000	13.844	91.605	79.548	36.171	-116.488	-25.554	1.862
3100	13.848	92.059	79.944	37.556	-116.802	-22.515	1.587
3200	13.852	92.498	[illegible]	38.941	-117.133	-19.472	1.330
3300	13.856	92.925	80.705	40.326	-117.479	-16.414	1.087
3400	13.859	93.338	81.070	41.712	-117.840	-13.342	0.858
3500	13.862	93.740	81.426	43.098	-118.216	-10.262	0.641
3600	13.864	94.131	81.774	44.484	[illegible]	-7.178	0.436
3700	13.867	94.511	82.113	45.871	-119.011	-4.074	0.241
3800	13.869	94.880	82.444	47.258	-119.430	-0.961	0.055
3900	13.871	95.241	82.768	48.645	-119.965	2.165	-0.121
4000	13.873	95.592	83.084	50.032	[illegible]	5.296	-0.289
4100	13.875	95.934	83.393	51.419	-120.781	8.446	-0.450
4200	13.877	96.269	83.696	52.807	-121.262	11.600	-0.604
4300	13.878	96.595	83.992	[illegible]	-121.760	14.771	-0.751
4400	13.880	96.914	84.282	55.582	-122.278	17.956	-0.892
4500	13.881	97.226	84.566	56.970	-122.811	21.150	-1.027
4600	13.882	97.532	84.845	58.359	-123.364	24.357	-1.157
4700	13.884	[illegible]	85.118	59.747	-123.939	27.570	-1.282
4800	13.885	98.122	85.386	61.135	-124.535	30.806	-1.403
4900	13.886	98.409	85.649	62.524	-125.153	34.045	-1.518
5000	13.887	98.689	85.907	63.912	-125.796	37.305	-1.631
5100	13.888	98.964	86.160	65.301	-126.465	40.576	-1.739
5200	13.889	99.234	86.409	66.690	-127.162	43.857	-1.843
5300	13.889	99.498	86.653	68.079	-127.889	47.159	-1.945
5400	13.890	99.758	86.894	69.468	-128.650	50.463	-2.042
5500	13.891	100.013	87.130	70.857	-129.445	53.796	-2.138
5600	13.892	100.263	87.362	72.246	-130.281	57.137	-2.230
5700	13.892	100.509	87.591	73.635	-131.160	60.500	-2.320
5800	13.893	100.751	87.816	75.024	-132.089	63.870	-2.407
5900	13.893	100.988	88.037	76.414	-133.072	67.266	-2.492
6000	13.894	101.222	88.255	77.803	-134.117	70.668	-2.574

15 September 1962 CHW

CHROMIUM DIOXIDE (CrO_2) (IDEAL MOLECULAR GAS) gfw = 84.01

ΔH^o_{f0} = -18.595 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = -19.000 kcal gfw^{-1}

Point Group = C_{2v}

$S^o_{298.15}$ = 61.856 cal deg K^{-1}gfw^{-1}

$H^o_{298.15}-H^o_0$ = 2.640 kcal gfw^{-1}

Vibrational Levels and Multiplicities

ω, cm^{-1}	ω, cm^{-1}
870 (1)	926 (1)
388 (1)	

Bond lengths and angles:

Cr-O distance = 1.627 Å

O-Cr-O angle = 107°

Product of moments of inertia:

$I_AI_BI_C$ = 3.40637 x $10^{-115}g^3cm^6$ σ - 2

Heat of Formation

Based on mass-spectrometric work of Grimley et al[1].

Heat Capacity and Entropy

Calculated using estimated spectroscopic constants.

Reference

1. Grimley, R. T. et al, J. Chem. Phys. 34, 664 (1961).

TABLE 138

CHROMIUM TRIOXIDE CONDENSED PHASE CrO_3

Reference State for Calculating ΔH_f°, ΔF_f°, and Log Kp: Solid Cr from 0° to 2148°K, Liquid Cr from 1967°K, Gaseous Cr from 2967 to 6800°K, Gaseous O_2, Solid CrO_3 from 0° to 470°K, Liquid CrO_3 from 470° to 800°K

T, °K	cal/°K gfw			Kcal/gfw			Log K_p
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	
0	0.000	0.000	INFINITE	-2.970	-140.288	-140.288	INFINITE
298.15	18.090	18.260	18.260	0.000	-141.400	-123.234	90.328
300	18.130	[illegible]	18.260	0.034	-141.396	-123.121	89.689
311.65	18.390	19.067	18.274	0.247	-141.374	-122.398	85.830
311.65	18.390	19.067	18.274	0.247	-141.375	-122.398	85.830
400	19.930	23.853	18.993	1.944	-141.135	-117.062	63.956
470	20.840	27.141	19.967	3.372	-140.914	-112.853	52.474
470	29.000	38.541	19.967	8.730	-135.556	-112.853	52.474
500	29.000	40.336	21.136	9.600	-135.201	-111.431	48.704
600	29.000	45.623	24.790	12.500	-134.085	-106.782	38.893
700	29.000	50.093	28.093	15.400	-133.010	-102.318	31.943
800	29.000	53.966	31.091	18.300	-131.998	-98.004	26.772

15 September 1962 CHW

CHROMIUM TRIOXIDE (CrO_3) (CONDENSED PHASE) gfw = 100.01

$\Delta H^o_{f298.15}$ = -141.400 kcal gfw^{-1}

$S^o_{298.15}$ = 18.260 cal deg K^{-1}gfw^{-1}

T_m = 470°K

ΔH_m - 5.358 kcal gfw^{-1}

$H^o_{298.15}-H^o_0$ = 2.970 kcal gfw^{-1}

$C^o_p = 18.12 + 7.80 \times 10^{-3}T - 2.10 \times 10^5 T^{-2}$ cal deg K^{-1}gfw^{-1} $\quad 298.15°K \leq T \leq 470°K$

C^o_p = 29.00 cal deg K^{-1}gfw^{-1} $\quad 470°K \leq T \leq 800°K$

Structure

See volume 1, this study (section IVB6.4.3) for details.

Heat of Formation

The value of Mah[1] adopted.

Heat Capacity and Entropy

An equation estimated in an analogous manner to that used for $CrO_{2(s)}$.

Melting and Vaporization

See volume 1, this study (section IVB6.4.3) for details.

Reference

1. Mah, A. D., J. Am. Chem. Soc. 76, 3363 (1954).

CHROMIUM TRIOXIDE IDEAL MOLECULAR GAS CrO_3

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Cr from 0° to 2148°K, Liquid Cr from 2148° to 2967°K, Gaseous Cr from 2967° to 6000°K, Gaseous O_2, Gaseous CrO_3

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (kcal/gfw)	ΔH_f° (kcal/gfw)	ΔF_f° (kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-3.108	-67.426	-67.426	INFINITE
298.15	13.881	64.500	64.500	0.000	-68.400	-64.020	46.926
300	13.916	64.586	64.500	0.026	-68.404	-63.993	46.616
311.65	14.104	65.201	64.566	0.198	-68.423	-63.825	44.756
311.65	14.104	65.201	64.566	0.198	-68.424	-63.825	44.756
400	15.533	68.824	65.067	1.503	-68.576	-62.491	34.142
500	16.663	72.419	66.187	3.116	-68.685	-60.956	26.643
600	17.441	75.530	67.491	4.824	-68.761	-59.402	21.636
700	17.984	78.262	68.839	6.596	-68.814	-57.840	18.057
800	18.371	80.690	70.171	8.415	-68.873	-56.268	15.371
900	18.654	82.871	71.463	10.267	-68.941	-54.689	13.280
1000	18.867	84.848	72.704	12.144	-69.036	-53.099	11.604
1100	19.029	86.654	73.892	14.039	-69.170	-51.499	10.231
1200	19.156	88.316	75.025	15.948	-69.353	-49.885	9.085
1300	19.257	89.853	76.108	17.869	-69.587	-48.253	8.112
1400	19.338	91.283	77.141	19.799	-69.863	-46.603	7.275
1500	19.404	92.620	78.129	21.736	-70.172	-44.933	6.546
1600	19.459	93.874	79.074	23.679	-70.514	-43.237	5.906
1648	19.481	94.445	79.509	24.615	-70.694	-42.416	5.625
1648	19.481	94.445	79.509	24.615	-71.494	-42.416	5.625
1700	19.505	95.055	79.980	25.628	-71.700	-41.499	5.335
1800	19.543	96.171	80.849	27.580	-72.131	-39.710	4.821
1900	19.576	97.224	81.683	29.536	-72.616	-37.894	4.359
2000	19.605	98.233	82.486	31.495	-73.147	-36.052	3.939
2088	19.626	99.077	83.166	33.222	-73.661	-34.408	3.601
2088	19.626	99.077	83.166	33.222	-74.011	-34.408	3.601
2100	19.629	99.191	83.259	33.457	-74.084	-34.178	3.557
2148	19.639	99.632	83.617	34.400	-74.354	-33.240	3.382
2148	19.639	99.632	83.617	34.400	-79.294	-33.240	3.382
2200	19.650	100.104	84.004	35.421	-79.472	-32.120	3.191
2300	19.669	100.976	84.723	37.387	-79.820	-29.960	2.847
2400	19.686	101.816	85.418	39.355	-80.174	-27.787	2.530
2500	19.700	102.619	86.090	41.324	-80.537	-25.598	2.238
2600	19.713	103.392	86.741	43.295	-80.904	-23.392	1.966
2700	19.724	104.137	87.371	45.266	-8[illegible]	-21.171	1.714
2800	19.734	104.854	87.983	47.239	-81.[illegible]	-18.936	1.478
2900	19.744	105.547	88.577	49.213	-82.[illegible]	-16.692	1.258
2966.82	19.749	105.997	88.964	50.536	-82.3[illegible]	-15.179	1.180
2966.82	19.749	105.997	88.964	50.536	-162.532	-15.179	1.180
3000	19.752	106.216	89.154	51.188	-162.592	-13.536	0.986
3100	19.762	106.864	89.714	53.164	-162.794	-8.553	0.603
3200	19.766	107.491	90.260	55.140	-163.015	-3.584	0.245
3300	19.774	108.100	90.792	57.117	-163.251	1.406	-0.093
3400	19.779	108.690	91.309	59.094	-163.507	6.399	-0.411
3500	19.784	109.264	91.814	61.073	-163.776	11.403	-0.712
3600	19.789	109.821	92.307	63.051	-164.[illegible]	16.409	-0.996
3700	19.793	110.363	92.787	65.030	-164.367	21.430	-1.266
3800	19.797	110.891	93.257	67.010	-164.685	26.452	-1.521
3900	19.801	111.405	93.716	68.990	-165.022	31.496	-1.765
4000	19.804	111.907	94.164	70.970	-165.375	36.532	-1.996
4100	19.808	112.396	94.603	72.951	-165.745	41.586	-2.217
4200	19.811	112.873	95.032	74.931	-166.134	46.649	-2.427
4300	19.814	113.339	95.453	76.913	-166.539	51.720	-2.629
4400	19.816	113.795	95.864	78.894	-166.968	56.808	-2.822
4500	19.819	114.240	96.268	80.876	-167.412	61.893	-3.006
4600	19.821	114.676	96.663	82.858	-167.880	67.004	-3.183
4700	19.823	115.102	97.051	84.840	-168.372	72.112	-3.353
4800	19.825	115.520	97.431	86.823	-168.886	77.242	-3.517
4900	19.827	115.928	97.805	88.805	-169.428	82.369	-3.674
5000	19.829	116.329	98.171	90.788	-169.996	87.520	-3.825
5100	19.831	116.722	98.531	92.771	-170.596	92.677	-3.971
5200	19.832	117.107	98.885	94.754	-171.229	97.843	-4.112
5300	19.834	117.484	99.232	96.737	-171.899	103.027	-4.248
5400	19.835	117.855	99.574	98.721	-172.609	108.221	-4.380
5500	19.836	118.219	99.909	100.704	-173.362	113.443	-4.508
5600	19.838	118.577	100.239	102.688	-174.167	118.664	-4.631
5700	19.839	118.928	100.564	104.672	-175.027	123.912	-4.751
5800	19.840	119.273	100.884	106.656	-175.953	129.166	-4.867
5900	19.841	119.612	101.198	108.640	-176.912	134.449	-4.980
6000	19.842	119.945	101.508	110.624	-178.035	139.740	-5.090

15 September 1962 CHW

CHROMIUM TRIOXIDE (CrO_3) (IDEAL MOLECULAR GAS) gfw = 100.01

ΔH^o_{f0} = -67.426 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = -68.400 kcal gfw^{-1}

Point Group = D_{3h}

$S^o_{298.15}$ = 64.500 cal deg $K^{-1} gfw^{-1}$

$H^o_{298.15} - H^o_0$ = 3.108 kcal gfw^{-1}

Vibrational Levels and Multiplicities

ω, cm^{-1}	ω, cm^{-1}
840 (1)	1023 (2)
397 (1)	374 (2)

Bond lengths and angles:

Cr-O distance = 1.627 Å

O-Cr-O angle = 120°

Product of moments of inertia:

$I_A I_B I_C = 2.34688 \times 10^{-114} g^3 cm^6$ $\sigma = 6$

Heat of Formation

Based on the mass-spectrometric data of Grimley *et al*[1]

Heat Capacity and Entropy

Calculated from estimated spectroscopic constants.

Reference

1. Grimley, R. T., R. P. Burns, and M. G. Inghram, J. Chem. Phys. 34, 664 (1961).

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Hf from 0° to 2495°K, Liquid Hf from 2495° to 4985°K, Gaseous Hf from 4985° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.435			
298.15	6.390	10.710	10.710	0.000			
300	6.400	10.750	10.710	0.012			
400	6.850	12.654	10.964	0.676			
500	7.162	14.215	11.460	1.378			
600	7.332	15.536	12.030	2.103			
700	7.502	16.678	12.613	2.845			
800	7.672	17.692	13.188	3.603			
900	7.842	18.605	13.740	4.379			
1000	8.011	19.440	14.269	5.172			
1100	8.181	20.212	14.774	5.981			
1200	8.350	20.931	15.258	6.807			
1300	8.519	21.607	15.721	7.652			
1400	8.689	22.244	16.164	8.512			
1500	8.859	22.850	16.590	9.389			
1600	9.028	23.427	16.999	10.284			
1700	9.198	23.979	17.394	11.195			
1800	9.368	24.510	17.774	12.123			
1900	9.537	25.021	18.142	13.069			
2000	9.707	25.514	18.459	14.031			
2033	9.764	25.673	18.614	14.352			
2033	9.764	26.485	18.614	16.032			
2100	9.877	26.803	18.870	16.660			
2200	10.046	27.267	19.241	17.656			
2300	10.216	27.717	19.600	18.669			
2400	10.386	28.155	19.947	19.699			
2495	10.547	28.562	20.268	20.694			
2495	8.000	30.662	20.268	25.933			
2500	8.000	30.678	20.289	25.973			
2600	8.000	30.991	20.694	26.773			
2700	8.000	31.293	21.081	27.573			
2800	8.000	31.584	21.451	28.373			
2900	8.000	31.865	21.805	29.173			
3000	8.000	32.136	22.145	29.973			
3100	8.000	32.398	22.472	30.773			
3200	8.000	32.652	22.786	31.573			
3300	8.000	32.899	23.089	32.373			
3400	8.000	33.137	23.381	33.173			
3500	8.000	33.[illegible]9	23.663	33.973			
3600	8.000	33.595	23.936	34.773			
3700	8.000	33.814	24.200	35.573			
3800	8.000	34.027	24.456	36.373			
3900	8.000	34.235	24.704	37.173			
4000	8.000	34.438	24.944	37.973			
4100	8.000	34.635	25.178	38.773			
4200	8.000	34.828	25.406	39.573			
4300	8.000	35.016	25.627	40.373			
4400	8.000	35.200	25.843	41.173			
4500	8.000	35.380	26.053	41.973			
4600	8.000	35.556	26.25[illegible]	42.773			
4700	8.000	35.728	26.457	43.573			
4800	8.000	35.896	26.652	44.373			
4900	8.000	36.061	26.842	45.173			
4985.40	8.000	36.200	27.001	45.856			
4985.40	8.885	62.936	27.001	179.152			
5000	8.898	62.962	27.106	179.282			
5100	8.988	63.139	27.811	180.176			
5200	9.078	63.315	28.492	181.080			
5300	9.1[illegible]	63.488	29.150	181.992			
5400	9.25[illegible]	63.661	29.788	182.913			
5500	9.337	63.831	30.405	183.842			
5600	9.419	64.000	31.004	184.780			
5700	9.500	64.167	31.584	195.726			
5800	9.578	64.333	32.147	186.680			
5900	9.653	64.498	32.695	187.641			
6000	9.725	64.661	33.226	188.610			

15 March 1963 HLS

$0^{\circ}K$ to $2495^{\circ}K$ Crystal
$2495^{\circ}K$ to $4985.40^{\circ}K$ Liquid
$4985.40^{\circ}K$ to $6000^{\circ}K$ Ideal Monatomic Gas

$\Delta H^{o}_{f0} = 0$

$\Delta H^{o}_{f298.15} = 0$

$\Delta H^{o}_{s298.15} = 144.924$ Kcal gfw^{-1}

$S^{o}_{298.15} = 10.710$ cal degK^{-1} gfw^{-1}

$T_t = 2033^{\circ}K$

$\Delta H_t = 1.650 \pm 0.200$ Kcal gfw^{-1}

$T_m = 2495^{\circ}K$

$\Delta H_m = 5.239 \pm 1.000$ Kcal gfw^{-1}

$T_b = 4985.40^{\circ}K$

$\Delta H_v = 133.296$ Kcal gfw^{-1}

$H^{o}_{298.15} - H^{o}_{0} = 1.435$ Kcal gfw^{-1}

$C^{o}_{p} = 6.3147 + 1.69646 \times 10^{-3}T$ cal degK^{-1}gfw^{-1} was used from 500° to $2495^{\circ}K$

Structure

H.C.P. up to $2033^{\circ}K$, B.C.C. from 2033° to $2495^{\circ}K$

Heat of Formation

Zero by definition

Heat Capacity and Entropy

Low-temperature data of Burk *et al*[1] was joined onto Fieldhouse and Lang's[2] high temperature data

Melting

See Barriault *et al*[3]

Heat of Sublimation

An average of two determinations. See volume I, this study (section IVA9) for details

References

1. Burk, D. L., I. Esterman and S. A. Friedberg, Z. Physik Chem. Neue Folge 16, 183 (1958).
2. Fieldhouse, I. B. and J. Lang, WADD TR-60-904 (July 1961) and private communication
3. Barriault, R. J. et al, Thermodynamics of Certain Refractory Compounds, Pt. I, Vol. I, ASD TR-61-260 (May 1962)

SUMMARY OF UNCERTAINTY ESTIMATES

T °K	C^{o}_{T}	S^{o}_{T}	$-(F^{o}_{T}-H^{o}_{298})/T$	$H^{o}_{T}-H^{o}_{298}$	ΔH_f	ΔF_f	Log K_f
	cal/°K gfw			Kcal/gfw			
298.15	±0.100	±0.050	±0.050	±0.000			
500	±0.100	±0.102	±0.061	±0.020			
500	±0.500	±0.102	±0.061	±0.020			
1000	±0.500	±0.448	±0.178	±0.270			
1500	±0.500	±0.651	±0.304	±0.520			
1500	±1.000	±0.651	±0.304	±0.520			
2000	±1.000	±0.939	±0.429	±1.020			
2033	±1.000	±0.955	±0.437	±1.053			
2033	±1.000	±1.053	±0.437	±1.253			
2495	±1.000	±1.258	±0.571	±1.715			
2495	±2.000	±1.659	±0.571	±2.715			
3000	±2.000	±2.028	±0.786	±3.725			
4000	±2.000	±2.603	±1.172	±5.725			
4985.40	±2.000	±3.043	±1.500	±7.696			

HAFNIUM IDEAL MONATOMIC GAS **Hf**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Hf from 0° to 2495°K, Liquid Hf from 2495° to 4985°K, Gaseous Hf from 4985° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.481	144.878	144.878	INFINITE
298.15	4.972	44.645	44.645	0.000	144.924	134.806	-98.811
300	4.973	44.675	44.645	0.009	144.921	134.743	-98.156
400	5.010	46.110	44.840	0.508	144.756	131.37[illegible]	-71.776
500	5.114	47.237	45.211	1.013	144.559	128.048	-55.967
600	5.285	48.184	45.629	1.533	144.354	124.765	-45.443
700	5.500	49.015	46.055	2.072	144.151	121.515	-37.937
800	5.734	49.764	46.472	2.634	143.955	118.297	-32.316
900	5.970	50.453	46.877	3.219	143.764	115.101	-27.949
1000	6.196	51.094	47.267	3.827	143.579	111.926	-24.460
1100	6.407	51.695	47.642	4.458	143.401	108.769	-21.609
1200	6.596	52.260	48.004	5.108	143.225	105.629	-19.237
1300	6.763	52.795	48.352	5.776	143.048	102.504	-17.232
1400	6.906	53.302	48.688	6.460	142.872	99.390	-15.515
1500	7.026	53.782	49.011	7.157	142.692	96.293	-14.029
1600	7.123	54.239	49.324	7.864	142.504	93.204	-12.730
1700	7.201	54.673	49.626	8.581	142.310	90.130	-11.586
1800	7.260	55.087	49.918	9.304	142.105	87.065	-10.571
1900	7.305	55.481	50.200	10.032	141.887	84.014	-9.663
2000	7.338	55.856	50.474	10.764	141.657	80.974	-8.848
2033	7.346	55.976	50.562	11.007	141.579	79.974	-8.597
2033	7.346	55.976	50.562	11.007	139.929	79.974	-8.597
2100	7.361	56.215	50.739	11.499	139.763	77.999	-8.117
2200	7.378	56.558	50.996	12.236	139.504	75.063	-7.456
2300	7.391	56.886	51.245	12.975	139.230	72.141	-6.855
2400	7.401	57.201	51.486	13.714	138.939	69.230	-6.304
2495	7.411	57.488	51.709	14.418	138.648	66.479	-5.823
2495	7.411	57.488	51.709	14.418	133.409	66.479	-5.823
2500	7.411	57.5[illegible]3	51.721	14.455	133.406	66.344	-5.800
2600	7.423	57.794	51.949	15.197	133.348	63.661	-5.351
2700	7.436	58.074	52.171	15.940	133.291	60.981	-4.936
2800	7.453	58.345	52.386	16.684	133.235	58.306	-4.551
2900	7.474	58.607	52.596	17.430	133.181	55.630	-4.192
3000	7.499	58.861	52.801	18.179	133.[illegible]30	52.956	-3.858
3100	7.530	59.107	53.000	18.930	133.0[illegible]	50.287	-3.545
3200	7.565	59.347	53.195	19.685	133.0[illegible]	47.615	-3.252
3300	7.606	59.580	53.385	20.444	132.995	44.947	-2.977
3400	7.653	59.808	53.571	21.207	132.958	42.278	-2.717
3500	7.704	60.030	53.752	21.974	132.925	39.613	-2.473
3600	7.761	60.248	53.929	22.748	132.899	36.949	-2.243
3700	7.822	60.462	54.103	23.527	132.878	34.283	-2.025
3800	7.889	60.671	54.273	24.317	132.863	31.619	-1.818
3900	7.959	60.877	54.440	25.105	132.856	28.954	-1.622
4000	8.033	61.079	54.603	25.904	132.855	26.288	-1.436
4100	6.111	61.279	54.764	26.711	132.862	23.621	-1.259
4200	8.191	61.475	54.921	27.526	132.877	20.961	-1.091
4300	8.275	61.669	55.076	28.350	132.901	18.293	-0.930
4400	8.360	61.860	55.228	29.[illegible]81	132.932	15.630	-0.776
4500	8.448	62.049	55.377	30.022	132.973	12.966	-0.630
4600	8.537	62.235	55.524	30.871	133.022	10.296	-0.489
4700	8.627	62.420	55.669	31.729	133.080	7.628	-0.355
4800	8.717	62.603	55.812	32.596	133.147	4.956	-0.226
4900	8.808	62.783	55.952	33.473	133.224	2.285	-0.102
4985.40	8.885	62.936	56.071	34.228	133.296	0.000	0.000
4985.40	8.885	62.936	56.071	34.228			
5000	8.898	62.962	56.091	34.358			
5100	8.988	63.139	56.227	35.252			
5200	9.078	63.315	56.362	36.156			
5300	9.166	63.488	56.494	37.068			
5400	9.252	63.661	56.626	37.989			
5500	9.337	63.841	56.755	38.918			
5600	9.419	64.000	56.883	39.856			
5700	9.500	64.167	57.009	40.802			
5800	9.578	64.333	57.134	41.756			
5900	9.653	64.498	57.258	42.717			
6000	9.725	64.661	57.380	43.686			

15 March 1963 HLS

HAFNIUM, MONATOMIC (Hf) (IDEAL GAS) gfw = 178.50

ΔH^{o}_{f0} = 144.878 Kcal gfw^{-1}

$\Delta H^{o}_{f298.15}$ = 144.924 Kcal gfw^{-1}

Ground State Configuration $^{3}F_{2}$

$S^{o}_{298.15}$ = 44.645 cal $degK^{-1}$ gfw^{-1}

$H^{o}_{298.15}-H^{o}_{0}$ = 1.481 Kcal gfw^{-1}

Electronic Levels and Multiplicities

Data from earlier report[1] using levels from Moore[2] were used.

Heat of Formation

Vapor-pressure data from two sources were used and averaged. Volume I, this report (section IVA9) contains additional details.

Heat Capacity and Entropy

Calculated on monatomic gas program

References

1. Barriault, R. J. et al, Thermodynamics of Certain Refractory Compounds, Pt. I, Vol. 1, ASD TR-61-260 (May 1962).
2. Moore, C., Atomic Energy Levels, Vol. 3, Nat. Bur. Std. (U.S.), Circ. 467 (1958)

HAFNIUM, MONATOMIC (Hf) (IDEAL GAS) GFW = 178.50

SUMMARY OF UNCERTAINTY ESTIMATES

	cal °K gfw			kcal gfw			
T, °K	C^{o}_{p}	S^{o}_{T}	$-(F^{o}_{T} - H^{o}_{298})/T$	$H_T - H^{o}_{298}$	ΔH_f	ΔF_f	Log K_p
298.15	±0.000	±0.002	±0.002	±0.000	±3.000		
1000	±0.001	±0.002	±0.003	±0.000			
2000	±0.001	±0.003	±0.003	±0.001			
2033	±0.001	±0.003	±0.003	±0.001			
2033	±0.001	±0.003	±0.003	±0.001			
2495	±0.001	±0.003	±0.003	±0.001			
2495	±0.001	±0.003	±0.003	±0.001			
3000	±0.001	±0.003	±0.003	±0.001			
4000	±0.003	±0.003	±0.003	±0.003			
5000	±0.006	±0.004	±0.003	±0.007			
6000	±0.011	±0.006	±0.003	±0.015			

HAFNIUM NITRIDE CONDENSED PHASE **HfN**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Hf from 0° to 2495°K, Liquid Hf from 2495° to 4985°K, Gaseous Hf from 4985° to 6000°K; Gaseous N_2; Solid HfN from 0° to 3583°K, Liquid HfN from 3583° to 6000°K

T, °K	cal/°K gfw C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	Kcal/gfw $H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.773	-87.542	-87.542	INFINITE
298.15	9.800	10.700	10.700	0.000	-88.240	-81.414	59.675
300	9.826	10.761	10.700	0.018	-88.240	-81.371	59.276
400	10.827	13.741	11.100	1.056	-88.215	-79.085	43.208
500	11.409	16.224	11.883	2.170	-88.154	-76.811	33.572
600	11.828	18.342	12.788	3.333	-88.073	-74.552	27.154
700	12.168	20.192	13.716	4.533	-87.978	-72.306	22.574
800	12.467	21.837	14.630	5.765	-87.876	-70.072	19.142
900	12.743	23.321	15.515	7.026	-87.771	-67.853	16.476
1000	13.003	24.677	16.364	8.313	-87.664	-65.645	14.346
1100	13.253	25.928	17.177	9.626	-87.554	-63.449	12.605
1200	13.497	27.092	17.956	10.964	-87.442	-61.262	11.157
1300	13.736	28.182	18.701	12.325	-87.337	-59.084	9.932
1400	13.972	29.209	19.415	13.711	-87.216	-56.916	8.885
1500	14.205	30.180	20.101	15.120	-87.099	-54.756	7.978
1600	14.436	31.105	20.760	16.552	-86.982	-52.604	7.185
1700	14.666	31.987	21.394	18.007	-86.857	-50.458	6.486
1800	14.895	32.831	22.007	19.485	-86.731	-48.322	5.867
1900	15.123	33.643	22.598	20.986	-86.603	-46.192	5.313
2000	[illegible]	34.424	23.170	22.509	-86.471	-44.067	4.815
2033	15.424	34.676	23.354	23.017	-86.426	-43.367	4.662
2033	15.424	34.676	23.354	23.017	-88.076	-43.367	4.662
2100	15.576	35.179	23.724	24.056	-87.983	-41.897	4.360
2200	15.802	35.909	24.261	25.625	-87.843	-43.005	4.272
2300	16.027	36.616	24.783	27.216	-87.699	-37.519	3.565
2400	16.253	37.303	25.290	28.830	-87.551	-35.342	3.218
2495	16.466	37.938	25.760	30.384	-87.407	-33.276	2.915
2495	16.466	37.938	25.760	30.384	-92.646	-33.276	2.915
2500	16.477	37.971	25.784	30.467	-92.625	-33.156	2.898
2600	16.702	38.622	26.266	32.126	-92.204	-30.789	2.588
2700	16.926	39.256	26.735	33.807	-91.762	-28.435	2.302
2800	17.151	39.876	27.193	35.511	-91.298	-26.097	2.037
2900	17.375	40.481	27.641	37.237	-90.814	-23.777	1.792
3000	17.599	41.074	28.079	38.986	-90.307	-21.475	1.564
3100	17.822	41.655	28.508	40.757	-89.778	-19.189	1.353
3200	18.046	42.224	28.927	42.550	-89.229	-16.918	1.155
3300	18.270	42.783	29.339	44.366	-88.657	-14.668	0.971
3400	18.493	43.332	29.742	46.204	-88.064	-12.434	0.799
3500	18.717	43.871	30.138	48.065	-87.449	-10.218	0.638
3583	18.902	44.412	30.462	49.626	-86.922	-8.396	0.512
3583	16.000	48.496	30.462	64.626	-71.922	-8.396	0.512
3600	16.000	48.574	30.547	64.898	-71.862	-8.093	0.491
3700	16.000	49.012	31.040	66.498	-71.509	-6.326	0.374
3800	16.000	49.439	31.519	68.098	-71.156	-4.570	0.263
3900	16.000	49.855	31.984	69.698	-70.804	-2.822	0.158
4000	16.000	50.260	32.435	71.298	-70.452	-1.084	0.059
4100	16.000	50.656	32.875	72.898	-70.101	0.644	-0.034
4200	16.000	51.040	33.303	74.498	-69.710	2.369	-0.123
4300	16.000	51.417	33.720	76.098	[illegible]	4.079	-0.207
4400	16.000	51.785	34.126	77.698	-69.050	5.788	-0.287
4500	16.000	52.144	34.523	79.298	-68.701	.482	-0.363
4600	16.000	52.476	34.910	.898	-68.352	9.167	-0.436
4700	16.000	52.840	35.287	82.498	-68.003	10.855	-0.505
4800	16.000	53.177	35.657	84.098	-67.655	12.526	-0.570
4900	16.000	53.507	36.018	85.698	-67.307	14.192	-0.633
4985.4	16.000	53.783	36.319	87.064	-67.010	15.613	-0.684
4985.4	16.000	53.783	36.319	87.064	-200.306	15.613	-0.684
5000	16.000	53.830	36.371	87.298	-200.268	16.240	-0.710
5100	16.000	54.147	36.716	88.898	-200.015	20.571	-0.881
5200	16.000	54.456	37.054	90.498	-199.772	24.896	-1.046
5300	16.000	54.762	37.385	92.098	-199.538	29.213	-1.205
5400	16.000	55.062	37.710	93.698	-199.313	33.527	-1.357
5500	16.000	55.355	38.028	95.298	-199.096	37.834	-1.503
5600	16.000	55.643	38.340	96.898	-198.889	42.145	-1.645
5700	16.000	55.927	38.660	98.498	-198.690	46.445	-1.781
5800	16.000	56.205	38.967	100.098	-198.499	50.740	-1.912
5900	16.000	56.476	39.241	101.698	-198.316	55.047	-2.039
6000	16.000	56.747	[illegible]	103.298	-198.141	59.333	-2.161

HAFNIUM NITRIDE (HfN) (CONDENSED PHASE) gfw = 192.508

$\Delta H_{f298.15}$ = -88.24 kcal gfw^{-1} $S^{o}_{298.15}$ = 10.7 cal $degK^{-1}gfw^{-1}$

T_m = 3583°K ΔH_m = 15.0 kcal gfw^{-1}

$H^{o}_{298.15}-H^{o}_{0}$ = 1.773 kcal gfw^{-1}

$C^{o}_{p} = 10.936 + 2.2268 \times 10^{-3}T - 1.5998 \times 10^{5}T^{-2}$ cal $degK^{-1}gfw^{-1}$ 298.15°K $\leq T \leq$ 3583°K

C^{o}_{p} = 16.0 cal $degK^{-1}$ gfw^{-1} 3583°K $\leq T \leq$ 6000°K

Structure

HfN has an fcc structure [NaCl (B1) type] with variable homogeneity range.

Heat of Formation

Combustion-calorimetry data of Humphrey[1] used.

Heat Capacity and Entropy

Low-temperature data estimated. High-temperature data of Neel *et al*[2] recalculated in present work and extrapolated to melting point.

Melting and Vaporization

Heat of fusion estimated.

References

1. Humphrey, G. L., J. Am. Chem. Soc. 75, 2806 (1953).
2. Neel, D. S. *et al*, WADD TR 60-924 (February 1962).

HAFNIUM MONOXIDE — IDEAL MOLECULAR GAS — HfO

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p Solid Hf from 0° to 2495°K, Liquid Hf from 2495° to 4985°K, Gaseous Hf from 4985° to 6000°K, Gaseous O_2, Gaseous HfO

T °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.108	19.360	19.360	INFINITE
298.15	7.471	57.736	57.736	0.000	18.996	12.281	-9.002
300	7.479	57.783	57.737	0.014	18.991	12.239	-8.916
400	7.911	59.994	58.035	0.784	18.742	10.024	-5.477
500	8.310	61.803	58.613	1.595	18.486	7.873	-3.441
600	8.671	63.351	59.277	2.444	18.232	5.773	-2.103
700	8.990	64.712	59.958	3.328	17.985	3.715	-1.160
800	9.265	65.931	60.630	4.241	17.741	1.695	-0.463
900	9.495	67.035	61.281	5.179	17.496	-0.296	0.072
1000	9.682	68.046	61.908	6.138	17.248	-2.260	0.494
1100	9.830	68.976	62.508	7.114	16.996	-4.198	0.834
1200	9.943	69.836	63.084	8.103	16.735	-6.113	1.113
1300	10.025	70.636	63.634	9.102	16.460	-8.006	1.346
1400	10.080	71.381	64.161	10.107	16.173	-9.878	1.542
1500	10.114	72.078	64.666	11.117	15.871	-11.728	1.709
1600	10.130	72.731	65.150	12.130	15.55[illegible]	-13.558	1.852
1700	10.131	73.345	65.614	13.143	15.211	-15.366	1.975
1800	10.122	73.924	66.060	14.155	14.851	-17.156	2.083
1900	10.103	74.471	66.488	15.167	14.470	-18.923	2.177
2000	10.079	74.988	66.900	16.176	14.067	-20.668	2.258
2033	10.070	75.153	67.033	16.508	13.929	-21.241	2.283
2033	10.070	75.153	67.033	16.508	12.279	-21.241	2.283
2100	10.050	75.479	67.297	17.182	11.991	-22.341	2.325
2200	10.018	75.946	67.680	18.186	11.543	-23.967	2.381
2300	9.983	76.391	68.049	19.186	11.072	-25.570	2.430
2400	9.948	76.815	68.406	20.182	10.577	-27.155	2.473
2495	9.914	77.200	68.733	21.1[illegible]6	10.086	-28.636	2.508
2495	9.914	77.200	68.733	21.126	4.847	-28.636	2.508
2500	9.912	77.220	68.750	21.175	4.832	-28.703	2.509
2600	9.876	77.608	69.083	22.165	4.557	-30.039	2.525
2700	9.840	77.980	69.406	23.151	4.273	-31.366	2.539
2800	9.805	78.338	69.719	24.133	3.984	-32.681	2.551
2900	9.771	78.661	70.022	25.112	3.689	-33.986	2.561
3000	9.739	79.012	70.316	26.087	3.388	-35.279	2.570
3100	9.707	79.331	70.602	2[illegible].[illegible]59	3.082	36.561	2.577
3200	9.676	79.638	70.879	28.029	2.771	37.834	2.584
3300	9.647	79.936	71.149	28.995	2.455	-39.097	2.589
3400	9.619	80.223	71.412	29.958	2.132	-40.353	2.594
3500	9.593	80.502	71.668	30.919	1.806	-41.598	2.597
3600	9.567	80.772	71.917	31.877	1.475	-42.832	2.600
3700	9.543	81.033	72.160	32.832	1.140	-44.059	2.602
3800	9.520	81.287	72.397	33.785	0.801	-45.275	2.604
3900	9.498	81.534	72.628	34.736	0.457	-46.483	2.605
4000	9.477	81.775	72.853	35.685	0.110	-47.682	2.605
4100	9.457	82.008	73.074	36.631	-0.242	-48.875	2.605
4200	9.437	82.236	73.289	37.576	-0.597	-50.052	2.604
4300	9.419	82.458	73.500	38.519	-0.956	-51.227	2.604
4400	9.402	82.674	73.706	39.460	-1.319	-52.390	2.602
4500	9.386	82.885	73.908	40.399	-1.[illegible]85	-53.548	2.601
4600	9.370	83.091	74.105	41.337	-2.055	-54.[illegible]96	2.599
4700	9.355	83.293	74.299	4[illegible].273	-2.430	-55.[illegible]37	2.596
4800	9.341	83.490	74.488	4[illegible].[illegible]08	-2.808	-56.966	2.594
4900	9.327	83.682	74.674	44.142	-3.191	-58.093	2.591
4985.40	9.316	83.843	74.829	44.938	-3.522	-59.043	2.588
4985.40	9.316	83.843	74.829	44.938	-136.818	-59.043	2.588
5000	9.314	83.870	74.856	45.074	-136.888	-58.819	2.571
5100	9.302	84.055	75.034	46.004	-137.377	-57.249	2.453
5200	9.290	84.235	75.209	46.934	-137.881	-55.671	2.340
5300	9.279	84.412	75.381	47.863	-138.400	-54.088	2.230
5400	9.268	84.585	75.550	48.790	-138.938	-52.489	2.124
5500	9.258	84.755	75.716	49.716	-139.494	-50.884	2.022
5600	9.248	84.922	75.879	50.641	-140.070	-49.265	1.923
5700	9.239	85.086	76.039	51.566	-140.667	-47.637	1.826
5800	9.230	85.246	76.196	52.489	-141.290	-45.996	1.733
5900	9.221	85.404	76.351	53.412	-141.939	-44.341	1.642
6000	9.213	85.559	76.503	54.334	-142.618	-42.678	1.554

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ΔH_{f0} = 19.360 kcal gfw^{-1}

$\Delta H_{f298.15}$ = 18.996 kcal gfw^{-1}

Ground-State Configuration = $^3\pi$

$S^\circ_{298.15}$ = 57.736 cal deg K^{-1} gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 2.108 kcal gfw^{-1}

State	g	E	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e \times 10^5$	$D_e \times 10^6$
		cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}
$^3\pi_2$	2	4003	895	---	---	0.3792	---	---	---
$^3\pi_1$	2	2084	895	---	---	0.3792	---	---	---
$^3\pi_0$	2	0	895	---	---	0.3792	---	---	---

Heat of Formation

A preliminary value based on the work of Ackermann and Thorn[1] has been used.

Heat Capacity and Entropy

Have been calculated using above spectroscopic constants.[2,3]

References

1. Ackermann, R. J. and R. J. Thorn, In: Progress in Ceramic Science, J. E. Burke, ed., Pergamon Press, New York (1961).
2. Krishnamurty, S. G., Proc. Phys. Soc. (London) 64A, 852 (1951).
3. Brewer, L. and M. S. Chandrasekharaiah, UCRL-8713 (June 1960).

TABLE 144

HAFNIUM DIOXIDE

CONDENSED PHASE

HfO_2

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Hf from 0° to 2495°K, Liquid Hf from 2495° to 4985°K, Gaseous Hf from 4985° to 6000°K, Solid HfO_2 from 0° to 3173°K, Liquid HfO_2 from 3173° to 6000°K

T °K	C_p° (cal/°K g fw)	S_T° (cal/°K g fw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K g fw)	$H_T^\circ - H_{298}^\circ$ (Kcal/g fw)	ΔH_f° (Kcal/g fw)	ΔF_f° (Kcal/g fw)	Log K_p
0	0.000	0.000	INFINITE	-2.345	-264.895	-264.895	INFINITE
298.15	14.400	14.188	14.188	0.000	-266.060	-252.486	185.068
300	14.447	14.277	14.188	0.027	-266.058	-252.401	183.865
400	16.167	18.700	14.780	1.568	-265.891	-247.873	135.425
500	17.079	22.414	15.945	3.234	-265.658	-243.395	106.383
600	17.673	25.583	17.294	4.974	-265.399	-238.968	87.040
700	18.117	28.342	18.680	6.764	-265.128	-234.586	73.237
800	18.482	30.786	20.043	8.594	-264.854	-230.239	62.895
900	18.799	32.982	21.361	10.459	-264.579	-225.929	54.860
1000	19.088	34.977	22.624	12.353	-264.306	-221.648	48.439
1100	19.358	36.810	23.832	14.276	-264.031	-217.397	43.191
1200	19.615	38.505	24.985	16.224	-263.757	-213.169	38.821
1300	19.863	40.085	26.086	18.198	-263.485	-208.964	35.128
1400	20.105	41.566	27.139	20.197	-263.210	-204.781	31.966
1500	20.341	42.961	28.148	22.219	-262.935	-200.616	29.228
1600	20.574	44.261	29.116	24.265	-262.661	-196.473	26.836
1700	20.804	45.535	30.045	26.334	-262.386	-192.343	24.726
1800	21.032	46.731	30.939	28.426	-262.111	-188.232	22.853
1900	21.258	47.874	31.800	30.540	-261.837	-184.134	21.179
1973	21.422	48.679	32.410	32.098	-261.636	-181.150	20.065
1973	26.000	49.946	32.410	34.598	-259.136	-181.150	20.065
2000	26.000	50.299	32.649	35.300	-258.939	-180.084	19.678
2033	26.000	50.725	32.939	36.158	-258.700	-178.785	19.219
2033	26.000	50.725	32.939	36.158	-260.350	-178.785	19.219
2100	26.000	51.568	33.520	37.900	-259.874	-176.106	18.327
2200	26.000	52.777	34.368	40.500	-259.181	-172.133	17.099
2300	26.000	53.933	35.194	43.100	-258.510	-168.193	15.981
2400	26.000	55.040	35.998	45.700	-257.862	-164.281	14.959
2495	26.000	56.049	36.742	48.170	-257.268	-160.586	14.066
2495	26.000	56.049	36.742	48.170	-262.507	-160.586	14.066
2500	26.000	56.101	36.781	48.300	-262.464	-160.382	14.020
2600	26.000	57.121	37.544	50.900	-261.596	-156.317	13.139
2700	26.000	58.102	38.287	53.500	-260.734	-152.285	12.326
2800	26.000	59.048	39.012	56.100	-259.876	-148.284	11.574
2900	26.000	59.960	39.719	58.700	-259.024	-144.315	10.875
3000	26.000	60.841	40.408	61.300	-258.176	-140.372	10.226
3100	26.000	61.694	41.081	63.900	-257.333	[illegible]36.455	9.620
3173	26.000	62.299	41.562	65.798	-256.721	[illegible]33.616	9.203
3173	26.000	70.178	41.562	90.798	-231.721	-133.616	9.203
3200	26.000	70.398	41.805	91.500	-231.495	-132.786	9.068
3300	26.000	71.198	42.683	94.100	-230.660	-129.711	8.590
3400	26.000	71.975	43.533	96.700	-229.830	-126.663	8.141
3500	26.000	72.728	44.357	99.300	-229.004	-123.642	7.720
3600	26.000	73.461	45.155	101.900	-228.182	-120.642	7.324
3700	26.000	74.173	45.930	104.500	-227.363	-117.668	6.950
3800	26.000	74.866	46.682	107.100	-226.548	-114.710	6.597
3900	26.000	75.542	47.414	109.700	-225.737	111.780	6.264
4000	26.000	76.200	48.125	112.300	-224.929	-108.868	5.948
4100	26.000	76.842	48.818	114.900	-224.125	-105.980	5.649
4200	26.000	77.469	49.492	117.500	-223.[illegible]25	-103.100	5.365
4300	26.000	78.080	50.150	120.100	-222.528	-100.246	5.095
4400	26.000	78.678	50.792	122.700	-221.736	-97.[illegible]12	4.838
4500	26.000	79.262	51.418	12[illegible].300	-220.947	-94.[illegible]	4.594
4600	26.000	79.834	52.030	127.900	-220.163	-91.798	4.361
4700	26.000	80.393	52.627	130.500	-219.384	-89.011	4.139
4800	26.000	80.940	53.211	133.100	-218.611	-86.242	3.927
4900	26.000	81.477	53.783	135.700	-217.844	-83.496	3.724
4985.40	26.000	81.926	54.261	137.921	-217.195	-81.156	3.558
4985.40	26.000	81.926	54.261	137.921	-350.491	-81.156	3.558
5000	26.000	82.002	54.342	138.300	-350.394	-80.370	3.513
5100	26.000	82.517	54.889	140.900	-349.738	-74.973	3.213
5200	26.000	83.022	55.425	143.500	-349.102	-69.588	2.925
5300	26.000	83.517	55.951	146.100	-348.487	-64.225	2.648
5400	26.000	84.003	56.466	148.700	-347.896	-58.862	2.382
5500	26.000	84.480	56.971	151.300	-347.330	-53.513	2.126
5600	26.000	84.948	57.466	153.900	-346.795	-48.170	1.880
5700	26.000	85.409	57.952	156.500	-346.293	-42.837	1.642
5800	26.000	85.861	58.430	159.100	-345.831	-37.517	1.414
5900	26.000	86.305	58.898	161.700	-345.413	-32.190	1.192
6000	26.000	86.742	59.359	164.300	-345.047	-26.882	0.979

15 June 196[illegible]

HLS

HAFNIUM DIOXIDE (HfO_2) (CONDENSED PHASE) gfw = 210.50

$\Delta H^\circ_{f298.15}$ = -266.060 kcal gfw^{-1}

$S^\circ_{298.15}$ = 14.188 cal deg K^{-1} gfw^{-1}

T_t = 1973°K

ΔH_t = 2.5 kcal gfw^{-1}

T_m = 3173°K

ΔH_m = 25.0 kcal gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 2.345 kcal gfw^{-1}

$C^\circ_p = 17.2346 + 2.1628 \times 10^{-3}T - 0.30930 \times 10^{6}T^{-2}$ cal degK^{-1} gfw^{-1} 298.15°K ≤ T ≤ 1973°K

C°_p = 26.0 cal deg K^{-1} gfw^{-1} 1973°K ≤ T ≤ 3173°K

C°_p = 26.0 cal deg K^{-1} gfw^{-1} 3173°K ≤ T ≤ 6000°K

Structure

Monoclinic from low temperature to 1973°K; tetragonal above 1973°K.

Heat of Formation

Heat-of-combustion determination is by Humphrey.[1]

Heat Capacity and Entropy

Low-temperature data are from Todd.[2] High-temperature data of Orr[3] have been joined to Todd data to 1973°K. Above 1973°K, data from Pears *et al*[4] have been used. Data above melting point have been estimated.

Melting and Vaporization

Transition and melting temperatures are from Curtis *et al.*[5] Heats of transition have been derived to be consistent with Orr[3] and Pears *et al.*[4] Heat of fusion is estimated.

References

1. Humphrey, G. L., J. Am. Chem. Soc. 75, 2806 (1953).
2. Todd, S. S., J. Am. Chem. Soc. 75, 3035 (1953).
3. Orr, R. L., J. Am. Chem. Soc. 75, 1231 (1953).
4. Pears, C. D. *et al.* ASD TDR 62-765 (January 1963).
5. Curtis, C. E., L. M. Doney, and J. R. Johnson, J. Am. Ceram. Soc. 37, 458 (1954).

HAFNIUM DIOXIDE (HfO_2) (CONDENSED PHASE) GFW = 210.50

SUMMARY OF UNCERTAINTY ESTIMATES

T °K	cal/°K gfw C°_p	S°_T	$-(F^\circ_T - H^\circ_{298})/T$	Kcal/gfw $H^\circ_T - H^\circ_{298}$	ΔH°_f	ΔF°_f	Log K_p
298.15	± 0.250	± 0.100	± 0.100	± 0.000	± 4.000		
500	± 0.250	± 0.229	± 0.128	± 0.050			
500	± 0.500	± 0.229	± 0.128	± 0.050			
1000	± 0.500	± 0.576	± 0.275	± 0.300			
1000	± 1.000	± 0.576	± 0.275	± 0.300			
1973	± 1.000	± 1.255	± 0.610	± 1.273			
1973	± 3.000	± 1.762	± 0.610	± 2.273			
2000	± 3.000	± 1.803	± 0.626	± 2.354			
3000	± 3.000	± 3.019	± 1.235	± 5.354			
3173	± 3.000	± 3.188	± 1.337	± 5.873			
3173	± 3.000	± 4.763	± 1.337	± 10.873			
4000	± 3.000	± 5.458	± 2.120	± 13.354			
5000	± 3.000	± 6.128	± 2.857	± 16.354			
6000	± 3.000	± 6.675	± 3.449	± 19.354			

HAFNIUM DIOXIDE

IDEAL MOLECULAR GAS

HfO_2

Reference State for Calculating ΔH_f°, ΔF_f°, and Log Kp Solid Hf from 0° to 2495°K, Liquid Hf from 2495° to 4985°K, Gaseous Hf from 4985° to 6000°K, Gaseous O_2, Gaseous HfO_2.

T, °K	cal/°K gfw			Kcal/gfw			
	C_p	S_T	$-(F_T - H_{298})/T$	$H_T - H_{298}$	ΔH_f	ΔF_f	Log K_p
0	0.000	0.000	INFINITE	-2.767	-69.257	-69.257	INFINITE
298.15	11.525	60.475	60.475	0.000	-70.000	-70.226	51.475
300	11.545	60.547	60.475	0.021	-70.004	-70.227	51.158
400	12.478	64.003	60.940	1.225	-70.174	-70.277	38.396
500	13.125	66.861	61.847	2.507	-70.325	-70.286	30.721
600	13.566	69.296	62.891	3.843	-70.470	-70.266	25.593
700	13.870	71.411	63.960	5.216	-70.616	-70.222	21.923
800	14.085	73.278	65.010	6.614	-70.774	-70.153	19.164
900	14.241	74.947	66.023	8.031	-70.947	-70.065	17.013
1000	14.358	76.454	66.992	9.461	-71.138	-69.956	15.288
1100	14.447	77.826	67.916	10.902	-71.345	-69.829	13.873
1200	14.516	79.087	68.795	12.350	-71.571	-69.681	12.690
1300	14.571	80.251	69.632	13.804	-71.819	-69.514	11.686
1400	14.615	81.332	70.429	15.264	-72.083	-69.327	10.822
1500	14.651	82.342	71.190	16.727	-72.367	-69.119	10.070
1600	14.681	83.288	71.917	18.194	-72.672	-68.894	9.410
1700	14.706	84.179	72.613	19.663	-72.997	-68.648	8.825
1800	14.727	85.020	73.279	21.135	-73.342	-68.384	8.303
1900	14.745	85.817	73.918	22.608	-73.709	-68.098	7.833
2000	14.760	86.574	74.532	24.084	-74.095	-67.790	7.407
2033	14.764	86.815	74.729	24.571	-74.227	-67.684	7.276
2033	14.764	86.815	74.729	24.571	-75.877	-67.684	7.276
2100	14.773	87.294	75.123	25.560	-76.154	-67.413	7.015
2200	14.785	87.982	75.692	27.038	-76.583	-66.986	6.654
2300	14.795	88.639	76.240	28.517	-77.033	-66.538	6.322
2400	14.803	89.269	76.770	29.997	-77.505	-66.074	6.017
2495	14.811	89.844	77.257	31.404	-77.974	-65.611	5.747
2495	14.811	89.844	77.257	31.404	-83.213	-65.611	5.747
2500	14.811	89.873	77.282	31.478	-83.226	-65.575	5.732
2600	14.818	90.454	77.778	32.959	-83.477	-64.865	5.452
2700	14.824	91.014	78.258	34.442	-83.732	-64.146	5.192
2800	14.830	91.553	78.723	35.924	-83.992	-63.414	4.949
2900	14.835	92.074	79.174	37.408	-84.256	-62.675	4.723
3000	14.839	92.577	79.613	38.891	-84.525	-61.927	4.511
3100	14.844	93.063	80.039	40.[illegible]75	-84.799	-61.165	4.312
3200	14.847	93.535	80.453	41.860	-85.075	50.400	4.125
3300	14.851	93.991	80.857	43.345	-85.355	[illegible]9.625	3.949
3400	14.854	94.435	81.250	44.830	-85.640	-58.841	3.782
3500	14.857	94.865	81.632	46.316	-85.928	-58.044	3.624
3600	14.859	95.284	82.006	47.801	-86.221	-57.245	3.475
3700	14.862	95.691	82.370	49.287	-86.516	-56.436	3.333
3800	14.864	96.088	82.726	50.774	-86.814	-55.617	3.199
3900	14.866	96.474	83.074	52.260	-87.117	-54.794	3.070
4000	14.868	96.850	93.413	53.747	-87.422	-53.960	2.948
4100	14.870	97.217	83.746	55.234	-87.731	-53.124	2.832
4200	14.871	97.576	84.071	56.721	-98.044	-52.272	2.720
4300	14.873	97.926	84.389	58.208	-88.360	-51.415	2.613
4400	14.874	98.267	84.700	59.695	-88.681	-50.548	2.511
4500	14.875	98.602	85.006	61.183	-89.004	-49.682	2.413
4600	14.877	98.929	85.305	62.670	-89.333	-48.8[illegible]3	2.319
4700	14.878	99.249	85.598	64.158	-89.666	-47.[illegible]5	2.228
4800	14.879	99.562	85.886	6[illegible]46	-90.005	-47.022	2.141
4900	14.880	99.869	86.168	67.[illegible]34	-90.350	-46.122	2.057
4985.40	14.881	100.126	86.405	68.405	-90.651	-45.347	1.988
4985.40	14.881	100.126	86.405	68.405	-223.947	-45.347	1.988
5000	14.881	100.169	86.445	68.622	-224.012	-44.825	1.959
5100	14.882	100.464	86.717	70.110	-224.468	-41.236	1.767
5200	14.883	100.753	86.984	71.598	-224.944	-37.635	1.582
5300	14.884	101.036	87.247	73.087	-225.440	-34.034	1.403
5400	14.884	101.315	87.505	74.575	-225.961	-30.413	1.231
5500	14.885	1[illegible].588	87.758	76.063	-226.507	-26.781	1.064
5600	14.886	101.856	88.007	77.552	-227.083	-23.139	0.903
5700	14.886	102.120	88.253	79.041	-227.692	-19.492	0.747
5800	14.887	102.378	88.494	80.529	-228.342	-15.828	0.596
5900	14.888	102.633	88.732	82.018	-229.035	-12.151	0.450
6000	14.888	102.883	88.965	83.507	-229.780	-8.458	0.308

15 September 1963 HLS

HAFNIUM DIOXIDE (HfO_2) (IDEAL MOLECULAR GAS) gfw = 210.50

ΔH°_{f0} = -69.257 kcal gfw^{-1}

$\Delta H^\circ_{f298.15}$ = -70.000 kcal gfw^{-1}

Point Group $D_{\infty h}$

$S^\circ_{298.15}$ = 60.475 cal $degK^{-1}$ gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 2.767 kcal gfw^{-1}

Vibrational Levels and Multiplicities

ω, cm^{-1}	ω, cm^{-1}
857.4 (1)	931.1 (1)
242.8 (2)	

Bond lengths and angles:

Hf-O distance = 1.74 A

O-Hf-O angle = 180°

Moments of inertia:

I = 16.085×10^{-39} gm cm^2 $\sigma = 2$

$B_e = 0.174$ cm^{-1}

Heat of Formation

Based primarily on observations of Shchukarev and Semenov[1].

Heat Capacity and Entropy

Estimated structural data was used to calculate properties on polyatomic gas computer program.

Reference

1. Shchukarev, S. A., and G. A. Semenov, Izv. V. U. Z. Khim. i Khim. Tekh. No. 5,845 (1962).

HAFNIUM DIOXIDE (HfO_2) (IDEAL MOLECULAR GAS) GFW = 210.50

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p	S°_T	$-(F^\circ_T - H^\circ_{298})/T$	$H^\circ_T - H^\circ_{298}$	ΔH°_f	ΔF°_f	Log K_p
	cal/°K gfw			kcal/gfw			
298.15	± 1.000	± 3.000	± 3.000	± 0.000	± 15.000		
1000	± 1.000	± 4.210	± 3.508	± 0.702			
2000	± 1.000	± 4.903	± 4.052	± 1.702			
3000	± 1.000	± 5.309	± 4.408	± 2.702			
4000	± 1.000	± 5.596	± 4.671	± 3.702			
5000	± 1.000	± 5.820	± 4.879	± 4.702			
6000	± 1.000	± 6.002	± 5.052	± 5.702			

IRIDIUM **Ir**

REFERENCE STATE

Reference State for Calculating ΔHf°, ΔFf°, and Log K_p: Solid Ir from 0° to 2700°K, Liquid Ir from 2700° to 4712°K, Gaseous Ir from 4712° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.274			
298.15	6.110	8.497	8.497	0.000			
300	6.117	8.535	8.498	0.011			
400	6.393	10.335	8.740	0.638			
500	6.598	11.784	9.208	1.288			
600	6.774	13.003	9.743	1.956			
700	6.936	14.060	10.286	2.642			
800	7.091	14.996	10.817	3.343			
900	7.243	15.840	11.329	4.060			
1000	7.391	16.611	11.819	4.792			
1100	7.538	17.322	12.287	5.539			
1200	7.685	17.985	12.735	6.300			
1300	7.830	18.605	13.162	7.075			
1400	7.974	19.191	13.572	7.866			
1500	8.118	19.746	13.966	8.670			
1600	8.262	20.275	14.344	9.489			
1700	8.406	20.780	14.708	10.323			
1800	8.549	21.264	15.058	11.170			
1900	[illegible]	21.710	15.397	12.032			
2000	8.835	22.160	15.725	12.909			
2100	8.978	22.614	16.043	13.799			
2200	9.121	23.035	16.351	14.704			
2300	9.263	23.444	16.651	15.623			
2400	9.406	23.841	16.942	16.557			
2500	9.549	24.228	17.226	17.505			
2600	9.691	24.605	17.502	18.467			
2700	9.833	24.973	17.772	19.442			
2700	10.000	27.273	17.772	25.652			
2800	10.000	27.637	18.118	26.652			
2900	10.000	27.988	18.453	27.652			
3000	10.000	28.328	18.777	28.652			
3100	10.000	28.655	19.090	29.652			
3200	10.000	28.972	19.393	30.652			
3300	10.000	29.280	19.688	31.652			
3400	10.000	29.576	19.974	32.652			
3500	10.000	29.868	20.253	33.652			
3600	10.000	30.150	20.524	34.652			
3700	10.000	30.424	20.788	35.652			
3800	10.000	30.691	21.046	36.652			
3900	10.000	30.950	21.296	37.652			
4000	10.000	31.204	21.541	38.652			
4100	10.000	31.450	21.779	39.652			
4200	10.000	31.692	22.013	40.652			
4300	10.000	31.927	22.240	41.652			
4400	10.000	32.157	22.464	42.652			
4500	10.000	32.381	22.681	43.652			
4600	10.000	32.601	22.894	44.652			
4700	10.000	32.816	23.103	45.652			
4711.55	10.000	32.844	23.130	45.768			
4711.55	7.556	62.974	23.130	187.[illegible]			
4800	7.567	[illegible]	23.863	188.397			
4900	7.579	63.268	24.665	189.154			
5000	7.592	63.421	25.438	189.913			
5100	7.605	63.572	26.185	190.672			
5200	7.618	63.719	26.905	191.434			
5300	7.632	63.865	27.602	192.196			
5400	7.646	64.007	28.274	192.960			
5500	7.661	64.148	28.925	193.725			
5600	7.676	64.286	[illegible]	194.492			
5700	7.692	64.422	30.166	195.261			
5800	7.708	64.556	30.758	196.031			
5900	7.726	64.688	31.332	196.802			
6000	7.744	64.818	31.889	197.576			

15 September 1962 RCF

0^oK to 2700^oK	Crystal
2700^oK to 4711.55^oK	Liquid
4711.55^oK to 6000^oK	Ideal Monatomic Gas

ΔH^o_{f0} = 0 kcal gfw^{-1} $\Delta H^o_{f298.15}$ = 0 kcal gfw^{-1}

$\Delta H^o_{s298.15}$ = 158.000 kcal gfw^{-1} $S^o_{298.15}$ = 8.497 cal deg K^{-1}gfw^{-1}

T_m = 2700^oK ΔH_m = 6.210 kcal gfw^{-1}

T_b = 4711.55^oK ΔH_v = 141.960 kcal gfw^{-1}

$H^o_{298.15}-H^o_0$ = 1.274 kcal gfw^{-1}

$C^o_p = 5.997 + 1.422 \times 10^{-3}T - 0.2763 \times 10^5 T^{-2}$ cal deg K^{-1}gfw^{-1}

$298.15^oK \leq T \leq 2700^oK$

C^o_p = 10.000 cal deg K^{-1}gfw^{-1} $2700^oK \leq T \leq 4711.55^oK$

Structure

An fcc (A1) type [1]

Heat of Formation

Zero by definition

Heat Capacity and Entropy

See volume 1, this study (section IVA10) for details.

Melting

An average of three determinations adopted.

Vaporization

An extrapolation of ΔF^o_f of the ideal gas to zero adopted

Reference

1. Owens, E. A and E L. Yates, Phil Mag 15, 472 (1933)

IRIDIUM (Ir) (REFERENCE STATE) GFW = 192.2

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S_T (cal/°K gfw)	$-(F_T - H_{298})/T$ (cal/°K gfw)	$H_T - H_{298}$ (Kcal/gfw)	ΔH_f (Kcal/gfw)	ΔF_f (Kcal/gfw)	Log K_p
298.15	±0.070	±0.040	±0.040	±0.000			
1000	±0.500	±0.390	±0.190	±0.200			
2000	±1.000	±0.900	±0.420	±0.950			
2700	±1.500	±1.270	±0.590	±1.810			
2700	±1.500	±1.640	±0.590	±2.810			
3000	±1.130	±1.730	±0.710	±3.070			
4000	±3.130	±2.340	±1.040	±5.200			
4711.55	±4.560	±2.970	±1.280	±7.940			
4711.55	±0.002	±0.003	±0.003	±0.003			
5000	±0.002	±0.003	±0.003	±0.003			
6000	±0.004	±0.004	±0.003	±0.006			

TABLE 147

IRIDIUM

IDEAL MONATOMIC GAS

Ir

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ir from 0° to 2700°K, Liquid Ir from 2700° to 4712°K, Gaseous Ir from 4712° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.481	157.793	157.793	INFINITE
298.15	4.969	45.242	46.242	0.000	158.000	146.746	-107.563
300	4.969	46.273	46.242	0.009	157.998	146.677	-106.849
400	4.976	47.703	46.437	0.506	157.868	142.921	-78.085
500	5.007	48.816	46.806	1.005	157.717	139.201	-60.842
600	5.075	49.734	47.219	1.509	157.553	135.514	-49.359
700	5.180	50.524	47.636	2.021	157.379	131.855	-41.165
800	5.314	51.224	48.042	2.546	157.203	128.220	-35.026
900	5.465	51.859	48.431	3.085	157.025	124.608	-30.258
1000	5.622	52.443	48.804	3.639	156.847	121.015	-26.447
1100	5.780	52.966	49.159	4.209	156.670	117.441	-23.332
1200	5.933	53.495	49.500	4.795	156.495	113.882	-20.740
1300	6.079	53.976	49.826	5.396	156.321	110.337	-18.548
1400	6.215	54.432	50.139	6.010	156.144	106.806	-16.672
1500	6.340	54.865	50.439	6.638	155.968	103.291	-15.049
1600	6.455	55.278	50.727	7.278	155.789	99.784	-13.629
1700	6.560	55.672	51.008	7.929	155.606	96.290	-12.378
1800	6.654	56.050	51.278	8.590	155.427	92.804	-11.267
1900	6.739	56.412	51.539	9.259	155.227	89.330	-10.275
2000	6.815	56.760	51.791	9.937	155.028	85.868	-9.383
2100	6.883	57.094	52.036	10.622	154.823	82.415	-8.577
2200	6.944	57.415	52.273	11.314	154.610	78.972	-7.845
2300	6.999	57.725	52.503	12.011	154.388	75.540	-7.178
2400	7.048	58.024	52.727	12.713	154.156	72.116	-6.567
2500	7.093	58.313	52.945	13.420	153.915	68.703	-6.006
2600	7.133	58.592	53.157	14.132	153.665	65.297	-5.489
2700	7.170	58.862	53.363	[illegible]	153.405	61.904	-5.011
2700	7.170	58.862	53.363	14.847	147.195	61.904	-5.011
2800	7.204	59.125	53.564	15.566	146.914	58.751	-4.585
2900	7.235	59.377	53.760	16.288	146.636	55.610	-4.191
3000	7.263	59.622	53.952	17.012	146.360	52.475	-3.823
3100	7.289	59.861	54.138	17.740	146.088	49.351	-3.479
3200	7.313	60.093	54.321	18.470	145.818	46.230	-3.157
3300	7.336	60.318	54.499	19.203	145.551	43.124	-2.856
3400	7.357	60.537	54.674	19.937	145.286	40.020	-2.572
3500	7.377	60.751	54.844	20.674	145.022	36.932	-2.306
3600	7.396	60.959	55.011	[illegible]	144.761	33.847	-2.055
3700	7.413	61.162	55.175	22.153	144.501	30.768	-1.817
3800	7.430	61.360	55.335	22.895	144.247	27.772	-1.593
3900	7.446	61.551	55.492	23.637	143.987	24.636	-1.380
4000	7.461	61.742	55.646	24.385	143.733	21.580	-1.179
4100	7.475	61.926	55.797	25.131	143.479	18.526	-0.987
4200	7.489	62.107	55.945	25.880	143.228	15.486	-0.806
4300	7.503	62.283	56.090	26.629	142.977	12.445	-0.632
4400	7.516	62.456	56.233	27.380	142.728	9.416	-0.468
4500	7.529	62.625	56.373	28.132	142.480	6.386	-0.310
4600	7.541	62.790	56.511	28.886	142.234	3.362	-0.160
4700	7.554	62.953	56.646	29.641	141.989	0.348	-0.016
4711.55	7.556	62.971	56.661	29.728	141.960	0.000	0.000
4711.55	7.556	62.971	56.661	29.728			
4800	7.567	63.112	56.779	30.397			
4900	7.579	63.268	56.910	[illegible]			
5000	7.592	63.421	57.039	31.913			
5100	7.605	63.572	57.165	32.672			
5200	7.618	63.719	57.290	33.434			
5300	7.632	63.865	57.413	34.196			
5400	7.646	64.007	57.533	34.960			
5500	7.661	64.148	57.652	35.725			
5600	7.676	64.286	57.770	36.492			
5700	7.692	64.422	57.885	37.261			
5800	7.708	64.556	57.999	38.031			
5900	7.726	64.688	58.111	38.802			
6000	7.444	64.818	58.222	39.576			

15 September 1962 RCF

ΔH^{o}_{f0} = 157.793 kcal gfw^{-1}

$\Delta H^{o}_{f298.15}$ = 158.000 kcal gfw^{-1}

Ground State Configuration = $^{4}F_{4\frac{1}{2}}$

$S^{o}_{298.15}$ = 4.969 cal deg K^{-1}gfw^{-1}

$H^{o}_{298.15}-H^{o}_{0}$ = 1.481 kcal gfw^{-1}

Electronic Levels and Multiplicities

Energy levels from Moore.[1]

Heat of Formation

Third-Law determination of the Panish and Reif data.[2]

Heat Capacity and Entropy

Obtained from the monatomic gas-computer program.

References

1. Moore, C., Nat. Bur. Stds. (U.S.), Circ. 467, Vol. 3 (1 May 1958).
2. Panish, M. B. and L. Reif, J. Chem. Phys. 34, 1915 (1961).

IRIDIUM, MONATOMIC (Ir) (IDEAL GAS) GFW = 192.2

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^{o}_{p} (cal °K gfw)	S_T (cal °K gfw)	$-(F^{o}_{T} - H^{o}_{298})/T$ (cal °K gfw)	$H^{o}_{T} - H^{o}_{298}$ (Kcal gfw)	ΔH_f (Kcal gfw)	ΔF_f (Kcal gfw)	Log K_p
298.15	± 0.000	± 0.002	± 0.002	± 0.000	± 1.000	± 1.010	± 0.740
1000	± 0.000	± 0.002	± 0.003	± 0.000	± 1.200	± 1.190	± 0.260
2000	± 0.001	± 0.003	± 0.003	± 0.001	± 1.950	± 1.850	± 0.200
2700	± 0.001	± 0.003	± 0.003	± 0.001	± 2.810	± 2.600	± 0.210
2700	± 0.001	± 0.003	± 0.003	± 0.001	± 3.810	± 2.600	± 0.210
3000	± 0.001	± 0.003	± 0.003	± 0.001	± 4.070	± 3.140	± 0.230
4000	± 0.001	± 0.003	± 0.003	± 0.002	± 6.200	± 5.170	± 0.280
4711.55	± 0.002	± 0.003	± 0.003	± 0.003	± 8.940	± 7.050	± 0.330
4711.55	± 0.002	± 0.003	± 0.003	± 0.003			
5000	± 0.002	± 0.003	± 0.003	± 0.003			
6000	± 0.004	± 0.004	± 0.003	± 0.006			

TABLE 148

IRIDIUM MONOXIDE

IDEAL MOLECULAR GAS

IrO

Reference State for Calculating ΔH_f^o, ΔF_f^o, and Log K_p: Solid Ir from 0° to 2700 °K, Liquid Ir from 2700° to 4712°K, Gaseous Ir from 4712° to 6000°K, Gaseous O_2, Gaseous IrO.

T, °K	C_p^o (cal/°K gfw)	S_T^o (cal/°K gfw)	$-(F_T^o - H_{298}^o)/T$ (cal/°K gfw)	$H_T^o - H_{298}^o$ (Kcal/gfw)	ΔH_f^o (Kcal/gfw)	ΔF_f^o (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.124	106.394	106.394	INFINITE
298.15	7.623	59.634	59.634	0.000	106.000	98.059	-71.876
300	7.631	59.681	59.634	0.014	105.996	98.010	-71.397
400	8.011	61.931	59.938	0.797	105.798	95.378	-52.110
500	8.270	63.749	60.524	1.612	105.597	92.796	-40.559
600	8.442	65.272	61.192	2.448	105.387	90.256	-32.874
700	8.558	66.583	61.871	3.299	105.164	87.750	-27.396
800	8.640	67.731	62.533	4.159	104.924	85.280	-23.296
900	8.698	68.753	63.168	5.026	104.667	82.840	-20.115
1000	8.742	69.671	63.774	5.898	104.392	80.429	-17.577
1100	8.775	70.506	64.348	6.774	104.103	78.046	-15.506
1200	8.801	71.271	64.894	7.653	103.797	75.691	-13.785
1300	8.821	71.976	65.412	8.534	103.474	73.362	-12.333
1400	8.837	72.630	65.904	9.417	103.134	71.059	-11.092
1500	8.850	73.241	66.373	10.301	102.779	68.780	-10.021
1600	8.861	73.812	66.821	11.187	102.407	66.524	-9.086
1700	8.870	74.350	67.248	12.073	102.019	64.292	-8.265
1800	8.878	74.857	67.657	12.960	101.61	62.084	-7.538
1900	8.884	75.337	68.048	13.849	101.193	59.901	-6.890
2000	8.890	75.793	68.424	14.738	100.756	57.740	-6.309
2100	8.895	76.227	68.785	15.627	100.302	55.601	-5.786
2200	8.899	76.641	69.133	16.516	99.831	53.483	-5.313
2300	8.903	77.036	69.468	17.407	99.344	51.388	-4.883
2400	8.906	77.415	69.792	18.297	98.840	49.311	-4.490
2500	8.909	77.779	70.104	19.188	98.320	47.259	-4.131
2600	8.911	78.128	70.406	20.079	97.782	45.226	-3.801
2700	8.914	78.465	70.698	20.970	97.229	43.216	-3.498
2700	8.914	78.465	70.698	20.970	91.019	43.216	-3.498
2800	8.916	78.789	70.981	21.[illegible]61	90.439	41.457	-3.236
2900	8.917	79.[illegible]2	71.256	22.753	89.857	39.716	-2.993
3000	8.919	79.404	71.523	23.645	89.272	37.997	-2.768
3100	8.921	79.697	71.782	24.537	88.686	36.298	-2.559
3200	8.922	79.980	72.033	25.429	88.097	34.619	-2.364
3300	8.923	80.254	72.278	26.321	87.507	32.958	-2.183
3400	8.924	80.521	72.517	27.214	86.914	31.314	-2.013
3500	8.925	80.780	72.749	28.106	86.319	29.688	-1.854
3600	8.926	81.031	72.976	28.999	85.724	28.076	-1.704
3700	8.927	81.276	73.197	29.891	85.125	26.483	-1.564
3800	8.928	81.514	73.413	30.784	84.526	24.906	-1.432
3900	8.929	81.746	73.623	31.677	83.924	23.349	-1.308
4000	8.929	81.972	73.829	32.570	83.32.	21.802	-1.191
4100	8.930	82.192	74.030	33.463	82.716	20.273	-1.081
4200	8.931	82.407	74.227	34.356	82.109	18.758	-0.976
4300	8.931	82.618	74.420	35.249	81.501	17.257	-0.877
4400	8.932	82.823	74.609	36.142	80.890	15.769	-0.783
4500	8.932	83.024	74.794	37.035	80.277	14.294	-0.694
4600	8.933	83.220	74.975	37.929	79.663	12.836	-0.610
4700	8.933	83.412	75.152	38.822	79.046	11.394	-0.530
4711.55	8.933	83.435	75.173	38.929	78.974	11.232	-0.521
4711.55	8.933	83.435	75.173	38.929	-62.986	11.232	-0.521
4800	8.933	83.600	75.326	39.715	-63.321	12.628	-0.575
4900	8.934	83.784	75.497	40.609	-63.700	14.[illegible]1	-0.634
5000	8.934	83.965	75.664	41.502	-64.087	15.[illegible]5	-0.691
5100	8.934	84.142	75.829	42.395	-64.478	17.408	-0.746
5200	8.935	84.315	75.990	43.289	-64.876	19.020	-0.799
5300	8.935	84.485	76.149	44.182	-65.282	20.641	-0.851
5400	8.935	84.652	76.305	45.076	-65.696	22.262	-0.901
5500	8.936	84.816	76.458	45.969	-66.120	23.899	-0.950
5600	8.936	84.977	76.609	46.863	-66.556	25.536	-0.997
5700	8.936	85.136	76.757	47.757	-67.008	27.192	-1.043
5800	8.936	85.290	76.903	48.650	-67.477	28.851	-1.087
5900	8.937	8[illegible].444	77.046	49.544	-67.964	30.521	-1.131
6000	8.937	[illegible].594	77.188	50.437	-68.478	32.194	-1.173

15 September 1962 RCF

ΔH^o_{f0} = 106.394 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 106.000 kcal gfw^{-1}

Ground State Degeneracy = 4

$S^o_{298.15}$ = 59.634 cal deg K^{-1}gfw^{-1}

$H^o_{298.15}-H^o_0$ = 2.124 kcal gfw^{-1}

State	g	E (cm^{-1})	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})	$\omega_e y_e$ (cm^{-1})	B_e (cm^{-1})	α_e (cm^{-1})	$\gamma_e \times 10^5$ (cm^{-1})	$D_e \times 10^6$ (cm^{-1})
X	4	0.0	790	---	---	0.335	---	---	---

Heat of Formation

Data of Schafer and Heitland adopted in compilation.[1]

Heat Capacity and Entropy

Determined from using spectroscopic contants. See volume 1, this study (section IVA10.4) for details.

Reference

1. Schafer, H. and H. J. Heitland, Z. Anorg. Allgem. Chem. 304, 249 (1960).

TABLE 149

MAGNESIUM

REFERENCE STATE

Mg

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Mg from 0° to 923°K, Liquid Mg from 923° to 1377°K, Gaseous Mg from 1377° to 6000°K.

T, °K	C_p (cal/°K gfw)	S_T (cal/°K gfw)	$-(F_T - H_{298})/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.195			
298.15	5.951	7.800	7.800	0.000			
300	5.957	7.836	7.800	0.011			
400	6.212	9.587	8.037	0.620			
500	6.490	11.001	8.492	1.254			
600	6.608	12.212	9.013	1.919			
700	7.137	13.286	9.548	2.616			
800	7.470	14.261	10.077	3.347			
900	7.807	15.160	10.393	4.110			
923	7.885	15.358	10.709	4.291			
923	7.800	17.662	10.709	6.418			
1000	7.800	18.287	11.268	7.019			
1100	7.800	19.030	11.940	7.799			
1200	7.800	19.709	12.560	8.579			
1300	7.800	20.333	13.134	9.359			
1376.37	7.800	20.778	13.545	9.960			
1376.37	4.968	43.102	13.545	40.700			
1400	4.968	43.188	14.035	40.814			
1500	4.968	43.531	15.990	41.311			
1600	4.968	43.851	17.721	41.808			
1700	4.968	44.153	19.268	42.305			
1800	4.968	44.437	20.659	42.801			
1900	4.968	44.705	21.917	43.298			
2000	4.969	44.960	23.062	43.795			
2100	4.969	45..02	24.111	44.292			
2200	4.970	45.434	25.075	44.789			
2300	4.972	45.655	25.965	45.286			
2400	4.974	45.866	26.790	45.783			
2500	4.978	46.069	27.557	4 .281			
2600	4.983	46.265	28.273	46.779			
2700	4.989	46.453	28.943	47.278			
2800	4.998	46.634	29.571	47.777			
2900	5.009	46.810	30.163	48.277			
3000	5.023	46.980	30.720	48.779			
3100	5.040	47.145	31.248	49.282			
3200	5.060	47.305	31.747	49.787			
3300	5.085	47.461	32.220	50.294			
3400	5.114	47.614	32.672	50.804			
3500	5.148	47.762	33.100	51.317			
3600	5.186	47.908	33.510	51.834			
3700	5.229	48.051	33.901	52.354			
3800	5.278	48.191	34.275	52.880			
3900	5.332	48.328	34.634	53.410			
4000	5.392	48.464	34.978	53.946			
4100	5.457	48.598	35.308	54.489			
4200	5.528	48.730	35.626	55.038			
4300	5.604	48.861	35.933	55.594			
4400	5.686	48.991	36.228	56.159			
4500	5.773	49.120	36.513	56.732			
4600	5.866	49.248	36.788	57.314			
4700	5.964	49.375	37.055	57.905			
4800	6.067	49.502	37.313	58.507			
4900	6.176	49.628	37.563	9.119			
5000	6.289	49.754	37.806	59.742			
5100	6.407	49.879	38.040	60.377			
5200	6.530	50.005	38.270	61.024			
5300	6.658	50.131	38.493	61.683			
5400	6.790	50.256	38.709	62.355			
5500	6.927	50.382	38.920	63.041			
5600	7.069	50.508	39.126	63.741			
5700	7.215	50.635	39.327	64.455			
5800	7.366	50.761	39.522	65.184			
5900	7.522	50.889	39.715	65.929			
6000	7.687	51.016	39.901	66.689			

15 September 1962 RCF

$0^{o}K$ to $923^{o}K$	Crystal
$923^{o}K$ to $1376.37^{o}K$	Liquid
$1376.37^{o}K$ to $6000^{o}K$	Ideal Monatomic Gas

ΔH^{o}_{f0} = 0 kcal gfw^{-1}

$\Delta H^{o}_{f298.15}$ = 0 kcal gfw^{-1}

$\Delta H^{o}_{s298.15}$ = 35.340 kcal gfw^{-1}

$S^{o}_{298.15}$ = 7.800 cal deg K^{-1}gfw^{-1}

T_m = 923°K

ΔH_m = 2.127 kcal gfw^{-1}

T_b = 1376.37°K

ΔH_v = 30.740 kcal gfw^{-1}

$H^{o}_{298.15}-H^{o}_{0}$ = 1.195 kcal gfw^{-1}

Structure

See Barriault *et al*[1] for further details.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

See Barriault *et al*[1] for further details.

Melting

See Barriault *et al*[1] for further details.

Vaporization

See Barriault *et al*[1] for further details.

Reference

1. Barriault, R. J. *et al*, Thermodynamics of Certain Refractory Compounds, Vol. 1, ASD TR 61-260, Pt. I (May 1962).

MAGNESIUM (Mg) (REFERENCE STATE) GFW = 24.32

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^{o}_{p} (cal/°K gfw)	S^{o}_{T} (cal/°K gfw)	$-(F^{o}_{T}-H^{o}_{298})/T$ (cal/°K gfw)	$H^{o}_{T}-H^{o}_{298}$ (Kcal/gfw)	ΔH_f (Kcal/gfw)	ΔF_f (Kcal/gfw)	Log K_p
298.15	±0.030	±0.030	±0.030	±0.000			
923	±0.060	±0.060	±0.020	±0.040			
923	±0.160	±0.090	±0.020	±0.070			
1376.37	±0.600	±0.210	±0.070	±0.200			
1376.37	±0.000	±0.002					
2000	±0.000	±0.002					
3000	±0.001	±0.002					
4000	±0.002	±0.003					
5000	±0.002	±0.003					
6000	±0.002	±0.003					

MAGNESIUM IDEAL MONATOMIC GAS Mg

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Mg from 0° to 923°K, Liquid Mg from 923° to 1377°K, Gaseous Mg from 1377° to 6000°K.

T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
	cal/°K gfw			Kcal/gfw			
0	0.000	0.000	INFINITE	-1.481	35.054	35.054	INFINITE
298.15	4.968	35.504	35.504	0.000	35.340	27.080	-19.849
300	4.968	35.535	35.504	0.009	35.338	27.029	-19.690
400	4.968	36.964	35.699	0.506	35.226	24.275	-13.263
500	4.968	38.073	36.067	1.003	35.089	21.553	-9.420
600	4.968	38.978	36.479	1.500	34.921	18.860	-6.869
700	4.968	39.744	36.892	1.996	34.720	16.199	-5.057
800	4.968	40.408	37.291	2.493	34.486	13.569	-3.707
900	4.968	40.993	37.671	2.990	34.220	10.970	-2.664
923	4.968	41.118	37.755	3.104	34.153	10.377	-2.457
923	4.968	41.118	37.755	3.104	32.026	10.377	-2.457
1000	4.968	41.516	38.029	3.487	31.808	8.580	-1.875
1100	4.968	41.990	38.368	3.984	31.525	6.269	-1.245
1200	4.968	42.422	38.688	4.481	31.242	3.986	-0.726
1300	4.968	42.820	38.991	4.977	30.958	1.726	-0.290
1376.37	4.968	43.102	39.210	5.360	30.740	0.000	0.000
1376.37	4.968	43.102	39.210	5.360			
1400	4.968	43.188	39.278	5.474			
1500	4.968	43.531	39.550	5.971			
1600	4.968	43.851	39.809	6.468			
1700	4.968	44.153	40.056	6.965			
1800	4.968	44.437	40.291	7.461			
1900	4.968	44.705	40.517	7.958			
2000	[illegible]	44.960	40.732	8.455			
2100	4.969	45.202	40.940	8.952			
2200	4.970	45.434	41.139	9.449			
2300	4.972	45.655	41.330	9.946			
2400	4.974	45.866	41.515	10.443			
2500	4.978	46.069	41.693	10.941			
2600	4.983	46.265	41.865	11. 39			
2700	4.989	46.453	42.032	11.938			
2800	4.998	46.634	42.193	12.437			
2900	5.009	46.810	42.349	12.937			
3000	5.023	46.980	42.500	13.439			
3100	5.040	47.145	42.648	13.942			
3200	5.060	47.305	42.791	14.447			
3300	5.085	47.461	42.930	14.954			
3400	5.114	47.614	43.065	15.464			
3500	5.148	47.762	43.197	15.977			
3600	5.186	47.908	43.326	16.494			
3700	5.229	48.051	43.452	17.014			
3800	5.278	48.191	43.575	17.540			
3900	5.332	48.328	43.695	18.070			
4000	5.392	48.464	43.813	18.606			
4100	5.457	48.598	43.928	19.149			
4200	5.528	48.730	44.040	19.698			
4300	5.604	48.861	44.151	20.254			
4400	5.686	48.991	44.260	20.819			
4500	5.773	49.120	44.366	21.392			
4600	5.866	49.248	44.471	21.974			
4700	5.964	49.375	44.574	22.565			
4800	6.067	49.502	44.675	23.167			
4900	6.176	49.628	44.775	23.779			
5000	6.289	49.754	44.873	24.402			
5100	6.407	49.879	44.970	25.037			
5200	6.530	50.005	45.066	25.684			
5300	6.658	50.131	45.160	26.343			
5400	6.790	50.256	45.253	27.015			
5500	6.927	50.382	45.346	27.701			
5600	7.069	50.508	45.437	28.401			
5700	7.215	50.635	45.527	29.115			
5800	7.366	50.761	45.616	29.844			
5900	7.522	50.889	45.704	30.589			
6000	7.682	51.016	45.792	31.349			

15 September 1962 RCF

ΔH^{o}_{f0} = 30.054 kcal gfw^{-1}

$\Delta H^{o}_{f298.15}$ = 35.340 kcal gfw^{-1}

Ground State Configuration = $^{1}S_{0}$

$S^{o}_{298.15}$ = 35.504 cal deg K^{-1}gfw^{-1}

$H^{o}_{298.15}-H^{o}_{0}$ = 1.481 kcal gfw^{-1}

Electronic Levels and Multiplicities

Energy levels from Moore.[1]

Heat of Formation

See Barriault *et al.*[2]

Heat Capacity and Entropy

See Barriault *et al.*[2]

References

1. Moore, C., NBS Circ. 467, Vol. 1 (15 June 1949).
2. Barriault, R. J. *et al*, Thermodynamics of Certain Refractory Compounds, ASD TR 61-260, Pt. I (May 1962).

MAGNESIUM, MONATOMIC (Mg) (IDEAL GAS) GFW = 24.32

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw C^{o}_{p}	S^{o}_{T}	$-(F^{o}_{T} - H^{o}_{298})/T$	Kcal gfw $H^{o}_{T} - H^{o}_{298}$	ΔH_{f}	ΔF_{f}	Log K_{f}
298.15	± 0.000	±0.002	±0.000	±0.000	± 0.250	± 0.260	± 0.190
923					± .290	± 0.270	± 0.060
923					± .320	± 0.270	± 0.060
1000	± 0.000	±0.002	±0.002	±0.000			
1376.37					± .450	± 0.350	± 0.060
2000	± 0.000	±0.002	±0.003	±0.001			
3000	± 0.001	±0.002	±0.003	±0.001			
4000	± 0.002	±0.003	±0.003	±0.002			
5000	± 0.002	±0.003	±0.003	±0.004			
6000	± 0.002	±0.003	±0.003	±0.005			

MAGNESIUM OXIDE — CONDENSED PHASE — MgO

Reference State for Calculating ΔH_f°, ΔF_f° and Log K_p: Solid Mg from 0° to 923°K, Liquid Mg from 923° to 1377°K, Gaseous Mg from 1377° to 4000°K, Gaseous O_2, Solid MgO from 0° to 3098°K, Liquid MgO from 3098° to 4000°K.

T, °K	C_p (cal/°K gfw)	S_T (cal/°K gfw)	$-(F_T - H_{298})/T$ (cal/°K gfw)	$H_T - H_{298}$ (Kcal/gfw)	ΔH_f (Kcal/gfw)	ΔF_f (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.235	-142.703	-142.703	INFINITE
298.15	8.906	6.439	6.439	0.000	-143.700	-135.988	99.677
300	8.939	6.495	6.440	0.017	-143.701	-135.941	99.028
400	10.148	9.252	6.807	0.978	-143.704	-133.351	72.856
500	10.854	11.599	7.538	2.031	-143.650	-130.770	57.157
600	11.323	13.622	8.387	3.141	-143.583	-128.199	46.694
700	11.656	15.394	9.263	4.291	-143.517	-125.640	39.225
800	11.905	16.967	10.130	5.469	-143.471	-123.090	33.625
900	12.098	18.381	10.970	6.670	-143.440	-120.544	29.271
923	12.135	18.683	11.154	6.949	-143.436	-119.955	28.402
923	12.135	18.683	11.154	6.949	-145.563	-119.955	28.402
1000	12.251	19.663	11.775	7.888	-145.546	-117.824	25.749
1100	12.375	20.837	12.547	9.119	-145.513	-115.054	22.858
1200	12.478	21.918	13.283	10.362	-145.474	-112.286	20.449
1300	12.565	22.921	13.987	11.614	-145.431	-109.524	18.412
1376.37	12.622	23.644	14.505	12.584	-145.394	-107.401	17.045
1376.37	12.622	23.644	14.505	12.584	-176.134	-107.401	17.045
1400	12.638	23.855	14.659	12.874	-176.058	-106.251	16.586
1500	12.701	24.729	15.301	14.141	-175.72[illegible]	-101.276	14.755
1600	12.756	25.550	15.916	15.414	-175.38[illegible]	-96.325	13.157
1700	12.804	26.325	16.506	16.692	-175.046	-91.393	11.749
1800	12.845	27.058	17.072	17.975	-174.70[illegible]	-86.481	10.500
1900	12.882	27.754	17.616	19.261	-174.361	-81.590	9.385
2000	12.915	28.415	18.139	20.551	-174.018	-76.716	8.383
2100	12.945	29.046	18.644	21.844	-173.675	-71.860	7.478
2200	12.971	29.644	19.131	23.140	-173.332	-67.020	6.658
2300	12.994	30.216	19.601	24.438	-172.989	-62.196	5.910
2400	13.016	30.760	20.055	25.739	-172.646	-57.385	5.225
2500	13.035	31.311	20.494	27.042	-172.30[illegible]	-52.589	4.597
2600	13.052	31.823	20.921	28.346	-171.965	-47.808	4.018
2700	13.068	32.316	21.334	29.652	-171.627	-43.040	3.484
2800	13.082	32.791	21.734	30.959	-171.290	-38.284	2.988
2900	13.095	33.251	22.124	32.268	-170.955	-33.539	2.527
3000	13.107	33.695	22.50[illegible]	33.579	-170.623	-28.807	2.099
3098	13.118	34.116	22.863	34.863	-170.300	-24.178	1.726
3098	14.600	40.048	22.463	53.363	-151.800	-24.178	1.706
3100	14.600	40.057	22.474	53.392	-151.79[illegible]	-24.094	1.699
3200	14.600	40.561	23.420	54.852	-151.316	-19.986	1.365
3300	14.600	41.010	23.946	56.312	-150.846	-15.891	1.052
3400	14.600	41.446	24.454	57.772	-150.381	-11.802	0.759
3500	14.600	41.869	24.946	59.232	-149.921	-7.737	0.483
3600	14.600	42.280	25.42[illegible]	60.692	-149.467	-3.676	0.223
3700	14.600	42.680	25.882	62.152	-149.017	0.367	-0.022
3800	14.600	43.069	26.329	63.612	-148.576	4.399	-0.253
3900	14.600	43.449	26.764	65.072	-148.140	8.418	-0.472
4000	14.600	43.819	27.186	66.532	-147.712	12.426	-0.679

15 December 1962 — RCF

$\Delta H^{o}_{f298.15}$ = -143.700 kcal gfw^{-1} $S^{o}_{298.15}$ = 6.439 cal deg K^{-1}gfw^{-1}

T_m = 3098°K ΔH_m = 18.5 kcal gfw^{-1}

$H^{o}_{298.15}-H^{o}_{0}$ = 1.235 kcal gfw^{-1}

C^{o}_{p} = 13.7146 - 4.494 x 10^{-5}T -1418T^{-1} cal deg K^{-1}gfw^{-1}

298.15°K $\leq$ T $\leq$ 3098°K

C^{o}_{p} = 14.6 cal deg K^{-1}gfw^{-1} 3098°K $\leq$ T $\leq$ 4000°K

Structure

An fcc (NaCl) type.

Heat of Formation

Based on data of Holley and Huber.[1]

Heat Capacity and Entropy

Several sources available. Analysis by the Nat. Bur. Stds. (U.S.)[2] used for low-and high-temperature data. The latter extrapolated to melting point from 1200°K. Liquid C_p estimated. Heat of fusion estimated.

References

1. Holley, C. E. and E. J. Huber, J. Am. Chem. Soc. 73, 5577 (1951).
2. Nat. Bur. Stds. (U.S.) Rept. 6484 (1959).

MAGNESIUM OXIDE (MgO) (CONDENSED PHASE) GFW = 40.32

SUMMARY OF UNCERTAINTY ESTIMATES

	cal/°K gfw			Kcal gfw			
T, °K	C^{o}_{p}	S^{o}_{T}	$-(F^{o}_{T} - H^{o}_{298})/T$	$H^{o}_{T} - H^{o}_{298}$	ΔH^{o}_{f}	ΔF^{o}_{f}	Log K_p
298.15	±0.050	±0.020	±0.020	±0.000	±0.500	±0.510	0.370
923					± .610	±0.580	0.140
923					± .640	±0.580	0.140
1000	±0.280	±0.160	±0.080	±0.080			
1376.37					± .900	±0.760	0.120
1376.37					±1.350	±0.760	0.120
2000	±0.940	±0.390	±0.180	±0.410	±1.560	±1.000	0.110
3098	±1.780	±0.570	±0.290	±0.860	±2.010	±1.620	0.110
3098	±1.000	±1.050	±0.290	±2.360	±3.510	±1.620	0.110
4000	±2.000	±1.440	±0.500	±3.750	±4.900	±2.820	0.150

MAGNESIUM OXIDE IDEAL MOLECULAR GAS MgO

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Mg from 0° to 923°K, Liquid Mg from 923° to 1377°K, Gaseous Mg from 3177° to 6000°K; Gaseous O_2, Gaseous MgO.

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-2.112	-10.980	-10.980	INFINITE
298.15	7.506	52.891	52.891	0.000	-11.100	-17.238	12.635
300	7.514	52.938	52.891	0.014	-11.104	-17.276	12.585
400	7.912	55.156	53.191	0.786	-11.296	-19.305	10.547
500	8.211	56.955	53.770	1.593	-11.488	-21.286	9.303
600	8.425	58.472	54.430	2.425	-11.699	-23.225	8.459
700	8.581	59.783	55.103	3.276	-11.934	-25.128	7.845
800	8.698	60.937	55.762	4.140	-12.200	-26.996	7.375
900	8.784	61.967	56.395	5.015	-12.495	-28.827	7.000
923	8.807	62.189	56.537	5.217	-12.568	-29.244	6.924
923	8.807	62.189	56.537	5.217	-14.695	-29.244	6.924
1000	8.862	62.897	57.000	5.897	-14.936	-30.449	6.654
1100	8.924	63.744	57.575	6.787	-15.245	-31.985	6.355
1200	8.977	64.523	58.122	7.682	-15.554	-33.493	6.100
1300	9.023	65.244	58.642	8.582	-15.863	-34.975	5.880
1376.37	9.056	65.764	59.026	9.278	-16.100	-36.106	5.730
1376.37	9.056	65.764	59.026	9.278	-46.840	-36.106	5.730
1400	9.066	65.914	59.138	9.486	-46.846	-35.922	5.607
1500	9.105	66.541	59.611	10.395	-46.869	-35.141	5.120
1600	9.141	67.130	60.063	11.307	-46.892	-34.360	4.693
1700	9.176	67.686	60.496	12.223	-46.915	-33.576	4.316
1800	9.210	68.211	60.910	13.142	-46.936	-32.789	3.981
1900	9.243	68.711	61.308	14.065	-46.957	-32.005	3.681
2000	9.275	[illegible]	61.690	14.991	-46.978	-31.218	3.411
2100	9.306	69.640	62.059	15.920	-46.999	-30.432	3.167
2200	9.338	70.074	62.414	16.852	-47.020	-29.643	2.945
2300	9.369	70.490	62.757	17.788	-47.039	-28.855	2.742
2400	9.401	70.890	63.088	18.726	-47.059	-28.064	2.555
2500	9.433	71.276	63.409	19.668	-47.079	-27.276	2.384
2600	9.465	71.647	63.719	20.613	-47.098	-26.483	2.226
2700	9.498	72.006	64.021	21.561	-47.118	-25.695	2.080
2800	9.531	72.353	64.313	22.512	-47.137	-24.904	1.944
2900	9.565	72.689	64.597	23.467	-47.156	-24.111	1.817
3000	9.600	73.016	64.874	24.425	-47.176	-23.324	1.699
3098	9.635	73.326	65.138	25.368	-47.195	-22.549	1.591
3098	9.635	73.326	65.138	25.368	-47.195	-22.549	1.591
3100	9.636	[illegible]	65.143	25.387	-47.195	22.528	1.588
3200	9.673	73.641	65.405	[illegible]	-47.215	21.738	1.485
3300	9.711	73.941	65.661	27.322	-47.236	-20.950	1.387
3400	9.750	74.233	65.911	28.295	-47.258	20.156	1.296
3500	9.791	74.518	66.155	29.272	-47.281	-19.369	1.209
3600	9.833	74.797	66.393	30.253	-47.306	-18.575	1.128
3700	9.876	75.06[illegible]	66.626	31.238	-47.331	-17.786	1.051
3800	9.921	75.345	66.854	32.228	-47.360	-16.996	0.977
3900	9.967	75.576	67.078	33.222	-47.390	-16.207	0.908
4000	10.014	75.852	67.297	34.221	-47.423	-15.418	0.842
4100	10.064	76.103	67.511	35.225	-47.460	-14.630	0.780
4200	10.114	76.349	67.722	36.234	-47.500	13.843	0.720
4300	10.167	76.591	67.929	37.248	-47.544	-13.052	0.663
4400	10.220	76.829	68.132	38.267	-47.594	-12.266	0.609
4500	10.276	77.063	68.332	39.292	-47.647	-11.483	0.558
4600	10.332	77.293	68.528	40.322	-47.707	-10.695	0.508
4700	10.391	77.520	68.721	41.359	-47.772	-9.906	0.461
4800	10.450	77.744	68.911	[illegible]	-47.846	[illegible]	0.415
4900	10.511	77.965	69.098	[illegible]	-47.927	-8.334	0.372
5000	10.573	78.182	69.282	44.502	-48.016	-7.545	0.330
5100	10.637	78.397	69.464	45.563	-48.115	-6.770	0.290
5200	10.701	78.610	69.643	46.629	-48.226	-5.978	0.251
5300	10.767	78.820	69.819	47.702	-48.349	-5.188	0.214
5400	10.834	7[illegible].027	69.993	48.782	-48.485	-4.404	0.178
5500	10.901	7[illegible].232	70.165	49.868	-48.637	-3.617	0.144
5600	10.970	79.436	70.335	50.962	-48.807	-2.832	0.111
5700	11.039	79.637	70.503	52.062	-48.996	-2.043	0.078
5800	11.110	79.836	70.669	53.168	-49.212	-1.260	0.047
5900	11.181	80.033	70.833	54.282	-49.453	-0.462	0.017
6000	11.252	80.229	70.995	55.403	-49.725	0.324	-0.012

15 December 1962 RCF

ΔH^o_{f0} = -10 980 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = -11.100 kcal gfw^{-1}

Ground State Configuration = $^3\Sigma$

$S^o_{298.15}$ = 52.891 cal deg K^{-1}gfw^{-1}

$H^o_{298.15}-H^o_0$ = 2.112 kcal gfw^{-1}

State	g	E (cm^{-1})	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e \times 10^5$	$D_e \times 10^6$
$X\,^3\Sigma$	3	0	902	13.0	—	0.625	0.009		1.2
$^3\Sigma$	3	26863.9	817	9.5	—	0.585	0.008	—	1.2
$X'\,^1\Sigma$	1	19200.	782.84	5.15	—	0.5711	0.005	—	1.22
$A\,^1\pi$	2	22694.4	664.4	3.91	—	0.5056	0.0046	—	1.2
$B\,^1\Sigma$	1	39204.7	824.1	4.76	—	0.5822	0.0045	—	1.2

Heat of Formation

Several values of the heat of dissociation of MgO had been reported. An intermediate value adopted. See valume 1, this study (section IVB12.4) for details.

Heat Capacity and Entropy

Calculated using above spectroscopic constants. Brewer and Porter's[1] analysis was given greatest weight.

Reference

1. Brewer, L. and R. Porter, J. Chem. Phys. 22, 1876 (1954).

TABLE 153

MAGNESIUM NITRIDE

CONDENSED PHASE

Mg_3N_2

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Mg from 0° to 923°K, Liquid Mg from 923° to 1377°K, Gaseous Mg from 1377° to 6000°K, Gaseous N_2; α - Mg_3N_2 from 0° to 823°K, β - Mg_3N_2 from 823° to 1061°K, γ - Mg_3N_2 from 1061° to 2500°K

T °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0							
298.15	24.986	22.400	22.400	0.000	-110.200	-96.255	70.554
300	25.000	22.555	22.400	0.046	-110.200	-96.169	70.056
400	25.730	29.847	23.390	2.583	-110.187	-91.494	49.987
500	26.460	35.667	25.282	5.192	-110.183	-86.822	37.948
600	27.190	40.555	27.431	7.875	-110.208	-82.149	29.921
700	27.920	44.801	29.615	10.630	-110.271	-77.468	24.185
800	28.650	48.577	31.754	13.459	-110.378	-72.774	19.880
823	28.818	49.392	32.235	14.120	-110.417	-71.700	19.039
823	29.600	49.659	32.235	14.340	-110.197	-71.700	19.039
900	29.600	52.306	33.841	16.619	-110.267	-68.086	16.533
923	29.600	53.053	34.311	17.300	-110.307	-67.011	15.866
923	29.600	53.053	34.311	17.300	-116.688	-67.011	15.866
1000	29.600	55.425	35.846	19.579	-116.808	-62.862	13.738
1061	29.600	57.178	37.023	21.384	-116.912	-59.596	12.275
1061	29.540	57.423	37.023	21.644	-116.652	-59.596	12.275
1100	29.540	58.489	37.765	22.796	-116.719	-57.471	11.418
1200	29.540	61.060	39.601	25.750	-116.906	-52.074	9.484
1300	29.540	63.424	41.344	28.704	-117.103	-46.665	7.845
1377	29.540	65.124	42.626	30.979	-117.263	-42.507	6.746
1377	29.540	65.124	42.626	30.979	-209.483	-42.507	6.746
1400	29.540	65.613	43.000	31.658	-209.335	-39.701	6.197
1500	29.540	67.651	44.576	34.612	-208.701	-27.609	4.022
1600	29.540	69.558	46.079	37.566	-208.074	-15.558	2.125
1700	29.540	71.348	47.513	40.520	-207.453	-3.540	0.455
1800	29.540	73.037	48.884	43.474	-206.836	8.441	-1.025
1900	29.540	74.634	50.198	46.428	-206.226	20.379	-2.344
2000	29.540	76.149	51.458	49.382	-205.621	32.286	-3.528
2100	29.540	77.591	52.668	52.336	-205.019	44.168	-4.596
2200	29.540	78.965	53.833	55.290	-204.421	56.022	-5.565
2300	29.540	80.278	54.954	58.244	-203.827	67.847	-6.447
2400	29.540	81.535	56.036	61.198	-203.235	79.646	-7.252
2500	29.540	82.741	57.080	64.152	-202.649	91.420	-7.992

15 June 1963

RED

MAGNESIUM NITRIDE (Mg_3N_2) (CONDENSED PHASE) gfw = 100.976

$\Delta H^\circ_{f298.15} = -110.2 \pm 0.275$ kcal gfw^{-1}

$S^\circ_{298.15} = 22.4$ cal deg K^{-1} gfw^{-1}

$T_{t1} = 823° \pm 3°K$

$\Delta H_{t1} = 0.220$ kcal gfw^{-1}

$T_{t2} = 1061° \pm 5°K$

$\Delta H_{t2} = 0.260$ kcal gfw^{-1}

$C^\circ_p = 22.81 + 7.30 \times 10^{-3}T$ cal deg K^{-1} gfw^{-1} $\quad 298.15°K \leq T \leq 823°K$

$C^\circ_p = 29.60$ cal deg K^{-1} gfw^{-1} $\quad 823°K \leq T \leq 1061°K$

$C^\circ_p = 29.54$ cal deg K^{-1} gfw^{-1} $\quad 1061°K \leq T \leq 2500°K$

Structure

Low-temperature or α-phase body-centered cubic D5-type: a = 9.95 kX (no crystallographic data exist for β and γ phases).

Heat of Formation

Mitchell's[1] value of -110.2 ± 0.275 kcal gfw^{-1} has been used for these calculations.

Heat Capacity and Entropy

Mitchell's[1] value of 22.4 has been used for the entropy; also, his heat-capacity data have been used.

Melting and Vaporization

Magnesium nitride decomposes on heating, and the data are conflicting; accordingly, the γ phase has been extrapolated to 2500°K.

Reference

1. Mitchell, D. W., Ind. Eng. Chem. 41, 2027 (1949).

MAGNESIUM NITRIDE (Mg_3N_2) (CONDENSED PHASE) GFW = 100.976

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal/gfw)	ΔH°_f (Kcal/gfw)	ΔF°_f (Kcal/gfw)	Log K_p
298.15	± 1.180	± 3.200	± 3.200	± 0.000	± 0.275		
500	± 1.180	± 3.810	± 3.334	± 0.238			
823	± 1.180	± 4.398	± 3.646	± 0.619			
823	± 1.780	± 4.505	± 3.646	± 0.707			
1000	± 1.780	± 4.852	± 3.829	± 1.022			
1061	± 1.780	± 4.957	± 3.891	± 1.131			
1061	± 1.040	± 5.097	± 3.891	± 1.279			
1500	± 1.040	± 5.457	± 4.300	± 1.736			
2000	± 1.040	± 5.756	± 4.628	± 2.256			
2500	± 1.040	± 5.988	± 4.878	± 2.776			

MANGANESE REFERENCE STATE Mn

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K : Solid Mn from 0° to 1517°K, Liquid Mn from 1517° to 2319°K, Gaseous Mn from 2319° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.194			
298.15	6.290	7.640	7.640	0.000			
300	6.301	7.679	7.640	0.012			
400	6.822	9.567	7.894	0.669			
500	7.244	11.135	8.390	1.373			
600	7.628	12.490	8.963	2.117			
700	7.993	13.694	9.554	2.898			
800	8.349	14.785	10.141	3.715			
900	8.700	15.788	10.713	4.568			
990	9.012	16.632	11.213	5.365			
990	8.983	17.168	11.213	5.896			
1000	8.990	17.259	11.273	5.985			
1100	9.056	18.119	11.857	6.888			
1200	9.122	18.909	12.412	7.797			
1300	9.188	19.642	12.941	8.712			
1374	9.237	20.152	13.315	9.394			
1374	10.700	20.552	13.315	9.943			
1400	10.700	20.752	13.452	10.221			
1410	10.700	20.829	13.504	10.328			
1410	11.300	21.138	13.504	10.764			
1500	11.300	21.837	13.983	11.781			
1517	11.300	21.964	14.072	11.973			
1517	11.000	24.272	14.072	15.473			
1600	11.000	24.857	14.616	16.386			
1700	11.000	25.524	15.238	17.486			
1800	11.000	26.153	15.827	18.586			
1900	11.000	26.748	16.387	19.686			
2000	11.000	27.312	16.919	20.786			
2100	11.000	27.849	17.427	21.886			
2200	11.000	28.360	17.912	22.986			
2300	11.000	28.849	18.377	24.086			
2318.80	11.000	28.939	18.463	24.295			
2318.80	5.006	51.688	18.463	77.048			
2400	5.018	51.861	19.588	77.454			
2500	5.040	52.066	20.884	77.956			
2600	5.067	52.264	22.086	78.462			
2700	5.101	52.456	23.208	78.970			
2800	5.142	52.642	24.255	79.482			
2900	5.193	52.824	25.238	79.999			
3000	5.253	53.001	26.161	80.521			
3100	5.322	53.174	27.029	81.050			
3200	5.403	53.344	27.848	81.586			
3300	5.495	53.512	28.624	82.131			
3400	5.598	53.677	29.358	82.685			
3500	5.713	53.841	30.055	83.251			
3600	5.841	54.004	30.718	83.828			
3700	5.981	54.166	31.350	84.419			
3800	6.133	54.327	31.952	85.025			
3900	6.297	54.489	32.528	85.646			
4000	6.473	54.650	33.079	86.285			
4100	6.661	54.813	33.608	86.941			
4200	6.859	54.975	34.114	87.617			
4300	7.068	55.139	34.601	88.313			
4400	7.287	55.304	35.070	89.031			
4500	7.515	55.471	35.522	89.771			
4600	7.751	55.638	35.957	90.534			
4700	7.995	55.808	36.377	91.322			
4800	8.244	55.979	36.785	92.134			
4900	8.500	56.151	37.178	92.971			
5000	8.759	56.325	37.558	93.834			
5100	9.022	56.502	37.927	94.723			
5200	9.288	56.679	38.287	95.638			
5300	9.554	56.859	38.636	96.580			
5400	9.821	57.040	38.975	97.549			
5500	10.088	57.222	39.305	98.545			
5600	10.352	57.407	39.627	99.567			
5700	10.614	57.592	39.941	100.615			
5800	10.873	57.779	40.246	101.689			
5900	11.127	57.967	40.546	102.789			
6000	11.376	58.156	40.837	103.914			

15 December 1962 RCF

MANGANESE (Mn) (REFERENCE STATE) gfw 54.94

0°K to 1517°K Crystal
1517°K to 2319°K Liquid
2319°K to 6000°K Ideal Monatomic Gas

$\Delta H_{f0}^{o} = 0$ $\Delta H_{f298.15}^{o} = 0$

$\Delta H_{s298.15}^{o}$ 67.000 kcal gfw^{-1} $S_{298.15}^{o} = 7.640$ cal deg K^{-1}gfw^{-1}

$T_t = 990°K$ $\Delta H_t = 0.531$ kcal gfw^{-1}

$T_t = 1374°K$ $\Delta H_t = 0.549$ kcal gfw^{-1}

$T_t = 1410°K$ ΔH_t 0.436 kcal gfw^{-1}

$T_m = 1517°K$ $\Delta H_m = 3.500$ kcal gfw^{-1}

$T_b = 2319°K$ $\Delta H_v = 52.753$ kcal gfw^{-1}

$H_{298.15}^{o} - H_0^{o}$ 1.194 kcal gfw^{-1}

C_p^{o} 5.704 + 3.380 x 10^{-3}T - 0.375 x $10^{5}T^{-2}$ cal deg K^{-1}gfw^{-1}

298.15°K $\leq$ T $\leq$ 990°K

C_p^{o} = 8.330 + 0.660 x 10^{-3}T cal deg K^{-1} gfw^{-1} 990°K $\leq$ T $\leq$ 1374°K

C_p^{o} = 10.700 cal deg K^{-1}gfw^{-1} 1374°K $\leq$ T $\leq$ 1410°K

C_p^{o} = 11.300 cal deg K^{-1}gfw^{-1} 1410°K $\leq$ T $\leq$ 1517°K

C_p^{o} = 11.000 cal deg K^{-1}gfw^{-1} 1517°K $\leq$ T $\leq$ 2319°K

Structure

Four modifications. Room-temperature form (α - Mn) has b.c.c.

Heat of Formation

Zero by definition

Heat Capacity and Entropy

Low-temperature data reported by several authors adopted. High-temperature data of Naylor[1,2] adopted and extrapolated to boiling point

Melting and Vaporization

Determination of Sully[3] adopted. Heat of vaporization calculated. See volume 1, this study (section IVA13) for details

References

1. Naylor, B. F., J. Chem. Phys. 13, 328 (1945)
2. Kelley, K. K., B. F. Naylor, and C. H. Shomate, U. S. Bur. Mines, Tech. Paper 686 (1946)
3. Sully, A. H., Manganese, Metallurgy of the Rare Metals 3, Butterworths, London (1955)

MANGANESE (Mn) (REFERENCE STATE) GFW = 54.94

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C_p^o (cal/°K gfw)	S_T^o (cal/°K gfw)	$-(F_T^o - H_{298}^o)/T$ (cal/°K gfw)	$H_T^o - H_{298}^o$ (Kcal/gfw)	ΔH_f^o (Kcal/gfw)	ΔF_f^o (Kcal/gfw)	Log K_p
298.15	±0.050	±0.040	±0.040	±0.000			
990	±0.050	±0.070	±0.050	±0.020			
990	±0.050	±0.150	±0.050	±0.100			
1374	±0.100	±0.180	±0.080	±0.130			
1374	±0.200	±0.230	±0.080	±0.210			
1410	±0.300	±0.240	±0.090	±0.220			
1410	±0.500	±0.290	±0.090	±0.280			
1517	±0.500	±0.320	±0.100	±0.330			
1517	±0.500	±0.650	±0.100	±0.830			
2000	±1.610	±0.950	±0.270	±1.350			
2318.80	±2.310	±1.230	±0.380	±1.980			
2318.80	±0.000	±0.002	±0.003	±0.000			
3000	±0.000	±0.002	±0.003	±0.001			
4000	±0.001	±0.003	±0.003	±0.001			
5000	±0.002	±0.003	±0.003	±0.002			
6000	±0.003	±0.003	±0.003	±0.004			

MANGANESE

IDEAL MONATOMIC GAS

Mn

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Mn from 0° to 1517°K, Liquid Mn from 1517° to 2319°K, Gaseous Mn from 2319° to 6000°K.

T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
	cal/°K gfw			Kcal/gfw			
0	0.000	0.000	INFINITE	-1.481	66.713	66.713	INFINITE
298.15	4.968	41.494	41.494	0.000	67.000	56.907	-41.712
300	4.968	41.525	41.494	0.009	66.997	56.844	-41.409
400	4.968	42.954	41.689	0.506	66.837	53.482	-29.220
500	4.968	44.063	42.057	1.003	66.630	50.167	-21.927
600	4.968	44.968	42.469	1.500	66.383	46.896	-17.081
700	4.968	45.734	42.882	1.996	66.098	43.670	-13.634
800	4.968	46.398	43.281	2.493	65.778	40.488	-11.060
900	4.968	46.983	43.660	2.990	65.422	37.348	-9.060
990	4.968	47.457	43.985	3.437	65.072	34.556	-7.628
990	4.968	47.457	43.985	3.437	64.541	34.556	-7.628
1000	4.968	47.506	44.019	3.487	64.502	34.254	-7.486
1100	4.968	47.980	44.358	3.984	64.096	31.249	-6.208
1200	4.968	48.412	44.678	4.481	63.684	28.281	-5.150
1300	4.968	48.810	44.981	4.977	63.265	25.348	-4.261
1374	4.968	49.085	45.195	5.345	62.951	23.197	-3.690
1374	4.968	49.085	45.195	5.345	62.402	23.197	-3.690
1400	4.968	49.178	45.268	5.474	62.253	22.458	-3.506
1410	4.968	49.213	45.295	5.524	62.196	22.175	-3.437
1410	4.968	49.213	45.295	5.524	6 .760	22.175	-3.437
1500	4.968	49.521	45.540	5.971	61.190	19.664	-2.865
1517	4.968	49.577	45.586	6.055	61.082	19.193	-2.765
1517	4.968	49.577	45.586	6.055	57.582	19.193	-2.765
1600	4.969	49.841	45.799	6.468	57.082	17.107	-2.337
1700	4.969	50.143	46.046	6.965	56.479	14.626	-1.880
1800	4.971	50.427	46.281	7.462	55.876	12.183	-1.479
1900	4.973	50.695	46.507	7.959	55.273	9.772	-1.124
2000	4.977	50.951	46.722	8.456	54.670	7.394	-0.808
2100	4.982	51.194	46.930	8.954	54.068	5.044	-0.525
2200	4.991	51.426	47.129	9.453	53.467	2.723	-0.270
2300	5.002	51.648	47.320	9.953	52.867	0.431	-0.041
2318.60	5.005	51.652	65.529	17.753	52.753	0.000	0.000
2318.60	5.005	51.652	65.529	17.753			
2400	5.018	51.861	47.505	10.454			
2500	5.040	52.066	47.684	10.956			
2600	5.067	5 .264	47.855	11.462			
2700	5.101	5 .456	48.023	11.970			
2800	5.142	52.642	48.184	12.482			
2900	5.193	52.824	48.341	12.999			
3000	5.253	53.001	48.494	13.521			
3100	5.322	53.174	48.642	14.050			
3200	5.403	53.344	48.786	14.586			
3300	5.495	53.512	48.927	15.131			
3400	5.598	53.677	49.064	15.685			
3500	5.713	53.841	49.198	16.251			
3600	5.841	54.004	49.330	16.828			
3700	5.981	54.166	49.458	17.419			
3800	6.133	54.327	49.584	18.025			
3900	6.297	54.489	49.708	18.646			
4000	6.473	54.650	49.829	19.285			
4100	6.661	54.813	49.949	19.941			
4200	6.859	54.975	50.067	20.617			
4300	7.068	55.139	50.183	21.313			
4400	7.287	55.304	50.297	22.031			
4500	7.515	55.471	50.410	22.771			
4600	7.751	55.638	50.522	23.534			
4700	7.995	55.808	50.633	24.322			
4800	8.244	55.979	50.742	25.134			
4900	8.500	56.151	50.851	25.971			
5000	8.759	56.325	50.959	26.834			
5100	9.022	56.502	51.066	27.723			
5200	9.288	56.679	51.172	28.638			
5300	9.554	56.859	51.278	29.580			
5400	9.821	57.040	51.383	30.549			
5500	10.088	57.222	51.487	31.545			
5600	10.352	57.407	51.591	32.567			
5700	10.614	57.592	51.695	33.615			
5800	10.873	57.779	51.798	34.689			
5900	11.127	57.967	51.901	35.789			
6000	11.376	58.156	52.004	36.914			

15 December 1962 RGF

ΔH°_{f0} = 66.713 kcal gfw^{-1}

$\Delta H^{\circ}_{f298.15}$ = 67.000 kcal gfw^{-1}

Ground State Configuration = $^{6}S_{2\frac{1}{2}}$

$S^{\circ}_{298.15}$ = 41.494 cal deg K^{-1}gfw^{-1}

$H^{\circ}_{298.15}-H^{\circ}_{0}$ = 1.481 kcal gfw^{-1}

Electronic Levels and Multiplicities

Spectroscopic energy levels from Moore.[1]

Heat of Formation

An average $\Delta H_{298.15}$ value determined from three calculations. See volume 1, this study (section IVA1 3) for details.

Heat Capacity and Entropy

Calculated on monatomic-gas computer program.

Reference

1. Moore, C., Nat. Bur. Stds. (U.S.) Circ. 467, Vol. II (August 1952).

MANGANESE, MONATOMIC (Mn) (IDEAL GAS) GFW = 54.94

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^{\circ}_T - H^{\circ}_{298})/T$ (cal/°K gfw)	$H^{\circ}_T - H^{\circ}_{298}$ (Kcal/gfw)	ΔH°_f (Kcal/gfw)	ΔF°_f (Kcal/gfw)	Log K_p
298.15	±0.000	±0.002	±0.002	±0.000	±0.300	±0.310	
990					± .320	±0.350	
990					± .400	±0.350	
1000	±0.000	±0.002	±0.002	±0.000			
1374					± .430	±0.410	
1374					± .510	±0.410	
1410					± .520	±0.430	
1410					± .580	±0.430	
1517					± .630	±0.450	
1517					±1.130	±0.450	
2000	±0.000	±0.002	±0.003	±0.000	±1.650	±0.840	
2318.80					±2.280	±1.180	
3000	±0.000	±0.002	±0.003	±0.001			
4000	±0.001	±0.003	±0.003	±0.001			
5000	±0.002	±0.003	±0.003	±0.002			
6000	±0.003	±0.003	±0.003	±0.004			

MANGANESE OXIDE — IDEAL MOLECULAR GAS — MnO

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Mn from 0° to 1517°K, Liquid Mn from 1517° to 2319°K, Gaseous Mn from 2319° to 6000°K, Gaseous O_2; Gaseous MnO

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.118	31.000	31.000	INFINITE
298.15	7.569	55.616	55.616	0.000	30.600	23.602	-17.300
300	7.577	55.663	55.616	0.014	30.595	23.558	-17.161
400	7.968	57.899	55.918	0.792	30.361	21.247	-11.608
500	8.247	59.709	56.501	1.604	30.104	18.998	-8.304
600	8.439	61.231	57.166	2.439	29.817	16.803	-6.120
700	8.573	62.542	57.843	3.290	29.499	14.658	-4.576
800	8.671	63.694	58.503	4.152	29.144	12.563	-3.432
900	8.744	64.719	59.138	5.023	28.755	10.512	-2.553
990	8.795	65.554	59.683	5.812	28.375	8.706	-1.922
990	8.795	65.554	59.683	5.812	27.844	8.706	-1.922
1000	8.801	65.644	59.743	5.900	27.801	8.513	-1.861
1100	8.846	66.485	60.318	6.783	27.362	6.606	-1.312
1200	8.884	67.256	60.865	7.669	26.915	4.738	-0.863
1300	8.915	67.968	61.384	8.559	26.461	2.909	-0.489
1374	8.936	68.461	61.751	9.220	26.122	1.578	-0.251
1374	8.936	68.461	61.751	9.220	25.573	1.578	-0.251
1400	8.943	68.630	61.878	9.452	25.414	1.126	-0.176
1410	8.943	68.694	61.927	9.542	[illegible]	0.951	-0.147
1410	8.945	68.694	61.927	9.542	24.917	0.951	-0.147
1500	8.967	69.248	62.349	10.348	24.314	-0.559	0.081
1517	8.971	69.348	62.426	10.501	24.201	-0.838	0.121
1517	8.971	69.348	62.426	10.501	20.701	-0.838	0.121
1600	8.988	69.827	62.799	11.246	20.169	-2.006	0.274
1700	9.008	70.373	63.229	12.145	19.527	-3.373	0.434
1800	9.026	70.888	63.640	13.047	18.884	-4.701	0.571
1900	9.043	71.377	64.035	13.951	18.241	-5.993	0.689
2000	9.059	71.841	64.414	14.856	17.596	-7.252	0.792
2100	9.075	72.284	64.778	15.762	16.949	-8.478	0.882
2200	9.090	72.707	65.129	16.671	16.303	-9.674	0.961
2300	9.105	73.111	65.467	17.580	15.653	-10.840	1.030
2318.80	9.108	73.185	65.529	17.753	15.530	-11.057	1.042
2318.80	9.108	73.185	65.529	17.753	-37.223	-11.057	1.042
2400	9.119	73.499	65.794	18.491	-37.265	-10.144	0.924
2500	9.134	73.872	66.110	19.404	-37.318	-9.011	0.788
2600	9.149	74.231	66.416	20.318	-37.376	-7.881	0.662
2700	9.164	74.576	66.712	21.234	-37.436	-6.745	0.546
2800	9.179	74.910	66.999	22.151	[illegible]	[illegible]	0.438
2900	9.195	75.233	67.278	23.070	[illegible]	-4.468	0.337
3000	9.211	75.545	67.549	23.990	[illegible]	-3.326	0.242
3100	9.228	75.848	67.812	24.912	-37.738	-2.181	0.154
3200	9.246	76.142	68.068	25.836	-37.831	-1.037	0.071
3300	9.264	76.427	68.317	26.761	-37.934	0.118	-0.008
3400	9.282	76.704	68.560	27.589	-38.045	1.270	-0.082
3500	9.302	76.974	68.797	28.618	-38.169	2.427	-0.152
3600	9.322	77.237	69.027	29.549	-38.304	3.584	-0.218
3700	9.343	77.493	69.255	30.482	-38.452	4.748	-0.280
3800	9.364	77.743	69.475	31.418	-38.615	5.917	-0.340
3900	9.387	77.987	69.691	32.355	-38.793	7.089	-0.397
4000	9.410	78.226	69.902	33.295	-38.988	8.266	-0.452
4100	9.433	78.459	70.107	34.237	[illegible]	9.456	-0.504
4200	9.458	78.686	70.311	35.182	-39.431	10.633	-0.553
4300	9.483	78.911	70.509	36.129	-39.682	11.826	-0.601
4400	9.509	79.130	70.703	37.079	-39.954	13.026	-0.647
4500	9.535	79.345	70.894	38.031	-40.247	14.229	-0.691
4600	9.562	79.556	71.081	38.987	-40.562	15.438	-0.733
4700	9.590	79.763	71.264	39.945	-40.903	16.655	-0.774
4800	9.618	79.967	71.445	40.905	-41.268	17.882	-0.814
4900	9.647	80.166	71.622	41.869	-41.658	19.112	-0.852
5000	9.677	80.363	71.796	42.836	-42.074	20.345	-0.889
5100	9.707	80.556	71.967	43.806	-42.518	21.588	-0.925
5200	9.738	80.746	72.135	44.779	-42.990	22.852	-0.960
5300	9.769	80.934	72.301	45.755	-43.492	24.115	-0.994
5400	9.801	81.118	72.464	46.734	-44.027	25.389	-1.027
5500	9.833	81.300	72.624	47.717	-44.592	26.676	-1.060
5600	9.865	81.479	72.782	48.703	-45.192	27.971	-1.092
5700	9.899	81.656	72.938	49.692	-45.827	29.278	-1.123
5800	9.932	81.830	73.091	50.686	-46.492	30.591	-1.153
5900	9.966	82.002	73.243	51.682	-47.213	31.922	-1.182
6000	10.001	82.172	73.392	52.683	-47.970	33.258	-1.211

15 December 1962 — RCF

ΔH^o_{f0} = 31.000 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 30.600 kcal gfw^{-1}

Ground State Degeneracy = 4

$S^o_{298.15}$ = 55.616 cal deg K^{-1}gfw^{-1}

$H^o_{298.15}-H^o_0$ = 2.118 kcal gfw^{-1}

		cm^{-1}							
State	g	E	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e x 10^5$	$D_e x 10^6$
X	4	0	839.55	4.79	—	0.499	—	—	0.71
A	2	17909.59	762.75	9.60	0.06	0.453	—	—	0.64

Heat of Formation

Based on DasSarma.[1]

Heat Capacity and Entropy

Calculated using above spectroscopic constants based on DasSarma[1] and Herzberg.[2]

References

1. Das Sarma, J. M., Z. Physik 157, 98 (1959).
2. Herzberg, G., Spectra of Diatomic Molecules, I., 2nd ed, Van Nostrand, N. Y. (1950).

MOLYBDENUM

REFERENCE STATE

Mo

Reference State for Calculating ΔH_f°, ΔF_f°, and Log Kp: Solid Mo from 0° to 2890°K, Liquid Mo from 2890° to 4965°K, Gaseous Mo from 4965°K to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.092			
298.15	5.680	6.830	6.830	0.000			
300	5.690	6.865	6.830	0.011			
400	5.970	8.545	7.057	0.595			
500	6.150	9.905	7.499	1.203			
600	6.280	11.035	7.993	1.825			
700	6.350	12.013	8.499	2.460			
800	6.440	12.868	8.993	3.100			
900	6.550	13.633	9.467	3.750			
1000	6.700	14.329	9.919	4.410			
1100	6.860	14.977	10.349	5.090			
1200	7.050	15.586	10.761	5.790			
1300	7.240	16.162	11.154	6.510			
1400	7.450	16.710	11.531	7.250			
1500	7.680	17.227	11.894	8.000			
1600	7.932	17.731	12.244	8.780			
1700	8.200	18.220	12.580	9.587			
1800	8.486	18.697	12.907	10.421			
1900	8.791	19.163	13.224	11.285			
2000	9.112	19.622	13.532	12.180			
2100	9.451	20.075	13.833	13.108			
2200	9.808	20.523	14.127	14.071			
2300	10.182	20.967	14.415	15.070			
2400	10.574	21.409	14.697	16.107			
2500	10.983	21.849	14.975	17.185			
2600	11.411	22.288	15.247	18.305			
2700	11.855	22.727	15.516	19.468			
2800	12.317	23.166	15.782	20.676			
2890	12.745	23.563	16.018	21.804			
2890	10.000	25.864	16.018	27.454			
2900	10.000	25.899	16.053	28.554			
3000	10.000	26.238	16.387	29.554			
3100	10.000	26.566	16.710	30.554			
3200	10.000	26.883	17.022	31.554			
3300	10.000	27.191	17.326	32.554			
3400	10.000	27.489	17.620	33.554			
3500	10.000	27.779	17.906	34.554			
3600	10.000	28.061	18.185	35.554			
3700	10.000	28.335	18.456	36.554			
3800	10.000	28.602	18.719	37.554			
3900	10.000	28.861	18.975	38.554			
4000	10.000	29.115	19.226	39.554			
4100	10.000	29.361	19.470	40.554			
4200	10.000	29.602	19.708	41.554			
4300	10.000	29.836	19.942	42.554			
4400	10.000	30.068	20.169	43.554			
4500	10.000	30.292	20.391	44.554			
4600	10.000	30.512	20.609	45.554			
4700	10.000	30.727	20.822	46.554			
4800	10.000	30.938	21.031	47.554			
4900	10.000	31.144	21.235	48.554			
4965	10.000	31.276	21.366	49.204			
4965	12.401	59.735	21.366	190.501			
5000	12.500	59.822	21.635	190.936			
5100	12.775	60.072	22.386	192.200			
5200	13.033	60.322	23.112	193.491			
5300	13.275	60.571	23.817	194.806			
5400	13.498	60.813	24.500	196.145			
5500	13.703	61.073	25.163	197.505			
5600	13.889	61.321	25.806	198.885			
5700	14.056	61.569	26.432	200.283			
5800	14.204	61.815	27.040	201.696			
5900	14.334	62.058	27.630	203.123			
6000	14.444	62.300	28.206	204.562			

May 1962 CHW

MOLYBDENUM (Mo) (REFERENCE STATE) gfw = 95.95

$0^{o}K$ to $2890^{o}K$ Crystal
$2890^{o}K$ to $4965^{o}K$ Liquid
$4965^{o}K$ to $6000^{o}K$ Ideal Monatomic Gas

$\Delta H^{o}_{f0} = 0$

$\Delta H^{o}_{f298.15} = 0$

$\Delta H^{o}_{s298.15} = 158.200 \text{kcal gfw}^{-1}$

$S^{o}_{298.15} = 6.83 \text{ cal degK}^{-1}\text{gfw}^{-1}$

$T_m = 2890^{o}K$

$\Delta H_m = 6.650 \text{ kcal gfw}^{-1}$

$T_b = 4965^{o}K$

$\Delta H_v = 141.300 \text{ kcal gfw}^{-1}$

$H^{o}_{298.15} - H^{o}_{0} = 1.092 \text{ kcal gfw}^{-1}$

$C^{o}_{p} = 6.026 - 0.217\text{x}10^{-3}T + 0.0880\text{x}10^{-5}T^2 \text{cal degK}^{-1}\text{gfw}^{-1}$ $1500^{o}K \leq T \leq 2890^{o}K$

Structure

Mo has a b.c.c. structure.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Low-temperature data from Stull and Sinke,[1] and Hultgren.[2] Data to 1500°K from Stull and Sinke.[1] Equation derived from range above 1500°K, based on Rasor and McClelland[3] data.

Melting

Melting temperature in agreement with several sources.

Vaporization

Vapor-pressure data of Edwards et al[4] used.

Further details by Barriault et al.[5]

References

1. Stull, D. R. and G. C. Sinke, Thermodynamic Properties of Elements, Am. Chem. Soc., Washington, D. C. (1956).
2. Hultgren, R. et al, Selected Values of Thermodynamic Properties of Metals and Alloys, Wiley, New York (1963).
3. Rasor, N. and J. McClelland, J. Phys. Chem. Solids 15, 17 (1960).
4. Edwards, J. W. et al, J. Am. Chem. Soc. 74, 1539 (1952).
5. Barriault, R. J. et al, ASD TR 61-260 (May 1962), Pt. 1.

MOLYBDENUM (Mo) (REFERENCE STATE) GFW = 95.95

SUMMARY OF UNCERTAINTY ESTIMATES

	cal/°K gfw			kcal gfw			
T, °K	C^{o}_{p}	S^{o}_{T}	$-(F^{o}_{T} - H^{o}_{298})/T$	$H^{o}_{T} - H^{o}_{298}$	ΔH^{o}_{f}	ΔF^{o}_{f}	Log K_p
298.15	±0.300	±0.100	±0.100	±0.000			
1000	±0.500	±0.600	±0.320	±0.280			
2000	±0.800	±1.050	±0.580	±0.930			
2890	±2.000	±1.570	±0.820	±2.180			
2890	±2.000	±1.920	±0.820	±3.180			
3000	±2.000	±1.990	±0.860	±3.400			
4000	±3.000	±2.170	±1.240	±5.900			
4965	±4.000	±3.470	±1.600	±9.270			
4965	±0.004	±0.003					
5000	±0.004	±0.003					
6000	±0.005	±0.004					

TABLE 158

MOLYBDENUM — IDEAL MONATOMIC GAS — **Mo**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Mo from 0° to 2890°K, Liquid Mo from 2890° to 4965°K, Gaseous Mo from 4965° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.481	157.811	157.811	INFINITE
298.15	4.968	43.462	43.462	0.000	158.200	147.278	-107.953
300	4.968	43.493	43.463	0.009	158.198	147.210	-107.237
400	4.968	44.922	43.657	0.506	158.111	153.560	-78.434
500	4.968	46.031	44.025	1.003	158.000	139.937	-61.163
600	4.968	46.937	44.437	1.500	157.875	136.334	-49.657
700	4.968	47.703	44.851	1.996	157.736	132.754	-41.446
800	4.968	48.366	45.249	2.493	157.593	129.195	-35.293
900	4.968	48.951	45.629	2.990	157.440	125.654	-30.512
1000	4.968	49.475	45.988	3.487	157.277	122.131	-26.690
1100	4.969	49.948	46.327	3.984	157.094	118.624	-23.567
1200	4.970	50.381	46.647	4.481	156.891	115.136	-20.968
1300	4.972	50.778	46.949	4.978	156.668	111.666	-18.772
1400	4.977	51.147	47.236	5.475	156.425	108.213	-16.892
1500	4.985	51.491	47.509	5.973	156.173	104.778	-15.265
1600	4.998	51.813	57.768	6.472	155.892	101.362	-13.845
1700	5.017	52.116	48.015	6.973	155.586	97.961	-12.593
1800	5.043	52.404	48.251	7.476	155.255	94.581	-11.483
1900	5.079	52.677	48.476	7.982	154.897	91.221	-10.492
2000	5.125	52.939	48.693	8.492	154.512	87.878	-9.602
2100	5.183	53.190	48.901	9.007	154.099	84.557	-8.799
2200	5.255	53.433	49.102	9.529	153.658	81.299	-8.076
2300	5.340	53.669	49.295	10.059	153.189	77.977	-7.409
2400	5.440	53.898	49.482	10.598	152.691	74.717	-6.804
2500	5.556	54.122	49.663	11.147	152.162	71.480	-6.327
2600	5.689	54.343	49.839	11.710	151.605	68.260	-5.738
2700	5.839	54.560	50.010	12.286	151.018	65.067	-5.267
2800	6.006	54.776	50.176	12.878	150.402	61.897	-4.831
2890	6.171	54.968	50.323	13.426	149.822	59.057	-4.466
2890	6.171	54.968	50.323	13.426	143.172	59.057	-4.466
2900	6.190	54.989	50.339	13.487	143.133	58.771	-4.429
3000	6.392	55.203	50.497	14.116	142.762	55.869	-4.070
3100	6.611	55.416	50.652	14.766	142.412	52.979	-3.735
3200	6.847	55.629	50.805	15.439	142.085	50.096	-3.421
3300	7.099	55.844	50.954	16.136	141.782	47.226	-3.128
3400	7.367	56.060	51.101	16.860	141.506	44.363	-2.852
3500	7.650	56.277	51.246	17.610	141.256	41.510	-2.592
3600	7.946	56.497	51.389	18.390	141.036	38.664	-2.347
3700	8.254	56.719	51.530	19.200	140.846	35.827	-2.116
3800	8.573	56.943	51.669	20.041	140.687	32.992	-1.897
3900	8.901	57.170	51.807	20.915	140.561	30.155	-1.690
4000	9.235	57.400	51.944	21.822	140.468	27.328	-1.493
4100	9.575	57.632	52.080	22.762	140.408	24.498	-1.306
4200	9.917	57.867	52.215	23.736	140.382	21.672	-1.128
4300	10.260	58.104	52.349	24.745	140.391	18.851	-0.958
4400	10.601	58.344	52.483	25.788	140.434	16.020	-0.796
4500	10.939	58.586	52.616	26.865	140.511	13.190	-0.641
4600	11.271	58.830	52.748	27.976	140.622	10.359	-0.492
4700	11.959	59.076	52.880	29.119	140.765	7.529	-0.350
4800	11.909	59.323	53.012	30.295	140.941	4.690	-0.214
4900	12.211	59.572	53.143	31.501	141.147	1.852	-0.083
4965	12.401	59.735	53.229	32.301	141.297	0.000	0.000
4965	12.401	59.735	53.229	32.301			
5000	12.500	59.822	53.271	32.736			
5100	12.775	60.072	53.405	34.000			
5200	13.033	60.322	53.536	35.291			
5300	13.275	60.573	53.666	36.606			
5400	13.498	60.823	53.796	37.945			
5500	13.703	61.073	53.926	39.305			
5600	13.889	61.321	54.056	40.685			
5700	14.056	61.569	54.186	42.083			
5800	14.204	61.815	54.315	43.496			
5900	14.334	62.058	54.444	44.923			
6000	14.444	62.300	54.573	46.362			

May 1962 — CHW

MOLYBDENUM (Mo) (IDEAL MONATOMIC GAS) gfw = 95.95

ΔH^o_{f0} = 157.811 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 158.200 kcal gfw^{-1}

Ground State Configuration = $^7S_3$

$S^o_{298.15}$ = 43.462 cal degK^{-1}gfw^{-1}

$H^o_{298.15} - H^o_0$ = 1.481 kcal gfw^{-1}

Electronic Levels and Multiplicities

Atomic energy levels from Moore.[1]

Heat of Formation

Calculated from vapor-pressure data of Edwards *et al.*[2]

Heat Capacity and Entropy

Calculated on monatomic gas-computer program.

Further details by Barriault *et al.*[3]

References

1. Moore, C., Atomic Energy Levels, Vol. III, Nat. Bur. Stds. (1958).
2. Edwards, J. *et al*, J. Am. Chem. Soc. 74, 1539 (1952).
3. Barriault, R. J. *et al*, ASD TR 61-260 (May 1962), Pt. 1.

MOLYBDENUM, MONATOMIC (Mo) (IDEAL GAS) GFW = 95.95

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal °K gfw)	S^o_T (cal °K gfw)	$-(F^o_T - H^o_{298})/T$ (cal °K gfw)	$H^o_T - H^o_{298}$ (kcal gfw)	ΔH_f (kcal gfw)	ΔF_f (kcal gfw)	Log K_p
298.15	±0.000	±0.002	±0.002	±0.000	±0.800	±0.830	±0.610
1000	±0.000	±0.002	±0.002	±0.000	±1.080	±1.120	±0.240
2000	±0.000	±0.002	±0.003	±0.000	±1.730	±1.970	±0.220
2890	±0.001	±0.003	±0.003	±0.001	±2.980	±3.180	±0.240
2890	±0.001	±0.003	±0.003	±0.001	±3.980	±3.180	±0.240
3000	±0.001	±0.003	±0.003	±0.001	±4.200	±3.390	±0.250
4000	±0.002	±0.003	±0.003	±0.002	±6.700	±5.770	±0.320
4965	±0.004	±0.003	±0.003	±0.004	±0.070	±8.760	±0.390
4965	±0.004	±0.003	±0.003	±0.004			
5000	±0.004	±0.003	±0.003	±0.004			
6000	±0.005	±0.004	±0.003	±0.008			

TABLE 159

MOLYBDENUM MONOXIDE IDEAL MOLECULAR GAS **MoO**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Mo from 0° to 2890°K, Liquid Mo from 2890° to 4965°K, Gaseous Mo from 4965° to 6000°K, Gaseous O_2, Gaseous MoO

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-2.116	87.413	87.413	INFINITE
298.15	7.542	54.587	54.587	0.000	87.400	80.467	-58.981
300	7.550	54.634	54.587	0.014	87.396	80.424	-58.586
400	7.932	56.861	54.888	0.789	87.232	78.124	-42.683
500	8.203	58.662	55.469	1.597	87.067	75.869	-33.161
600	8.388	60.175	56.130	2.427	86.897	73.643	-26.823
700	8.515	61.478	56.803	3.272	86.718	71.448	-22.306
800	8.604	62.621	57.461	4.129	86.537	69.278	-18.925
900	8.669	63.639	58.092	4.992	86.342	67.133	-16.301
1000	8.717	64.555	58.693	5.862	86.138	65.010	-14.207
1100	8.754	65.387	59.264	6.735	85.912	62.906	-12.498
1200	8.783	66.150	59.807	7.612	85.665	60.827	-11.078
1300	8.806	66.854	60.322	8.492	85.396	58.767	-9.879
1400	8.824	67.508	60.812	9.373	85.105	56.729	-8.855
1500	8.839	68.117	61.279	10.256	84.804	54.714	-7.971
1600	8.851	68.689	61.725	11.141	84.470	52.717	-7.200
1700	8.861	69.225	62.150	12.027	84.108	50.743	-6.523
1800	8.870	69.731	62.557	12.913	83.715	48.794	-5.924
1900	8.877	70.211	62.948	13.800	83.291	46.862	-5.390
2000	8.883	70.667	63.322	14.688	82.834	44.958	-4.913
2100	8.889	71.100	63.683	15.577	82.342	43.073	-4.482
2200	8.893	71.514	64.029	16.466	81.813	41.219	-4.095
2300	8.898	71.909	64.363	17.356	81.246	39.385	-3.742
2400	8.901	72.288	64.686	18.246	80.637	37.579	-3.422
2500	8.904	72.651	64.997	19.136	79.985	35.800	-3.129
2600	8.907	73.001	65.298	20.027	79.290	34.047	-2.862
2700	8.910	73.337	65.590	20.917	78.549	32.314	-2.615
2800	8.912	73.661	65.872	21.809	77.761	30.621	-2.390
2890	8.914	73.943	66.119	22.611	77.009	29.117	-2.202
2890	8.914	73.943	66.119	22.611	70.359	29.117	-2.202
2900	8.914	73.974	66.146	22.700	70.300	28.980	-2.184
3000	8.916	74.276	66.412	23.591	69.715	27.564	-2.008
3100	8.918	74.568	66.671	24.483	69.129	26.167	-1.845
3200	8.919	74.852	66.922	25.375	68.540	24.790	-1.693
3300	8.921	75.126	67.166	26.267	67.949	23.433	-1.552
3400	8.922	75.392	67.404	27.159	67.3[illegible]7	22.093	-1.420
3500	8.923	75.651	67.636	[illegible]8.051	66.7[illegible]	20.766	-1.297
3600	8.924	75.902	67.862	28.944	66.16[illegible]	19.465	-1.182
3700	8.925	76.147	68.083	29.836	65.567	18.178	-1.074
3600	8.926	76.385	68.298	30.729	64.967	16.906	-0.972
3900	8.927	76.617	68.509	31.621	64.365	15.639	-0.876
4000	8.928	76.843	68.714	32.514	63.762	14.408	-0.787
4100	8.928	77.063	68.915	33.407	63.157	13.177	-0.702
4200	8.929	77.278	69.112	34.300	62.550	11.966	-0.623
4300	8.930	77.489	69.304	35.193	61.941	10.776	-0.548
4400	8.930	77.694	69.493	36.086	61.330	9.583	-0.476
4500	8.931	77.895	69.677	36.979	60.718	8.415	-0.409
4600	8.931	78.091	69.858	37.872	60.103	7.263	-0.345
4700	8.932	78.283	70.035	38.765	59.485	6.124	-0.285
4800	8.932	78.471	70.209	39.658	59.865	4.992	-0.227
4900	8.933	78.655	70.379	40.551	58.241	3.886	-0.173
4965	8.933	78.773	70.488	41.132	57.834	3.168	-0.139
4965	8.933	78.773	70.488	41.132	-83.463	.168	-0.139
5000	8.933	78.836	70.547	1.445	-83.767	3.775	-0.165
5100	8.933	79.012	70.711	42.338	-84.663	5.534	-0.237
5200	8.934	79.186	70.872	43.231	-85.591	7.311	-0.307
5300	8.934	79.356	71.031	44.125	-86.549	9.111	-0.376
5400	8.934	79.523	71.186	45.018	-87.539	10.930	-0.442
5500	8.935	79.687	71.340	45.912	-88.557	12.760	-0.507
5600	8.935	79.848	71.490	46.805	-89.608	14.610	-0.570
5700	8.935	80.006	71.638	47.699	-90.688	16.484	-0.632
5800	8.935	80.162	71.784	48.592	-91.800	18.380	-0.693
5900	8.936	80.314	71.927	49.486	-92.943	20.278	-0.751
6000	8.936	80.465	72.068	50.379	-94.122	22.218	-0.809

May 1962 CHW

MOLYBDENUM MONOXIDE (MoO) (IDEAL MOLECULAR GAS) gfw = 111.95

$\Delta H^\circ_{f0} = 87.413$ kcal gfw^{-1}

$\Delta H^\circ_{f298.15} = 87.400$ kcal gfw^{-1}

Ground State Configuration = $^1\Sigma$

$S^\circ_{298.15} = 54.587$ cal degK^{-1} gfw^{-1}

$H^\circ_{298.15} - H^\circ_0 = 2.116$ kcal gfw^{-1}

		cm^{-1}							
State	g	E	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e \times 10^5$	$D_e \times 10^6$
$^1\Sigma$	1	0.0	840	-	-	0.41076	-	-	-

Heat of Formation

Based on mass spectrometric observations of De Maria et al[1]

Heat Capacity and Entropy

Calculated using above estimated spectroscopic constants. Further details by Barriault, et al.[2]

References

1. De Maria G. et al, J. Chem. Phys. 32, 1373 (1960).
2. Barriault, R. J., et al, ASD TR 61-260 (May 1962), Pt. 1.

TABLE 160

MOLYBDENUM DIOXIDE CONDENSED PHASE MoO_2

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Mo from 0° to 2890°, Liquid Mo from 3890° to 4965°K, Gaseous Mo from 4965° to 6000°K; Gaseous O_2; Solid MoO_2.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.995	-139.628	-139.628	INFINITE
298.15	13.380	11.060	11.060	0.000	-140.800	-127.450	93.419
300	13.421	11.143	11.060	0.025	-140.799	-127.367	92.782
400	15.075	15.232	11.607	1.450	-140.668	-122.906	67.150
500	16.148	18.730	12.690	3.020	-140.437	-118.489	51.789
600	16.996	21.774	13.957	4.690	-140.145	-114.128	41.569
700	17.739	24.468	15.268	6.440	-139.807	-109.817	34.285
800	18.425	26.898	16.573	8.260	-139.425	-105.559	28.836
900	19.079	29.112	17.845	10.140	-139.009	-101.350	24.610
1000	19.712	31.145	19.075	12.070	-138.567	-97.189	21.240
1100	20.332	33.022	20.258	14.040	-138.116	-93.073	18.491
1200	20.943	34.781	21.398	16.060	-137.644	-89.000	16.208
1300	21.547	36.429	22.491	18.120	-137.161	-84.968	14.284
1400	22.147	37.992	23.542	20.230	-136.655	-80.972	12.640
1500	22.743	39.503	24.556	22.420	-136.085	-77.013	11.220
1600	22.337	41.007	25.538	24.750	-135.412	-73.096	9.984
1700	23.929	42.565	26.494	27.320	-134.532	-69.231	8.900
1800	24.519	44.256	27.434	30.280	-133.295	-65.425	7.943
1900	25.108	46.180	28.369	33.840	-131.493	-61.701	7.097
2000	25.695	48.457	29.317	38.280	-128.848	-58.094	6.348

May 1962 CHW

MOLYBDENUM DIOXIDE (MoO_2) (CONDENSED PHASE) gfw = 127.95

$\Delta H^o_{f298.15}$ = -139.628 kcal gfw^{-1} $S^o_{298.15}$ = 11.060 cal degK^{-1}gfw^{-1}

$H^o_{298.15} - H^o_0$ = 1.995 kcal gfw^{-1}

$C^o_p = 14.11 + 5.82\times10^{-3}T - 2.18\times10^5T^{-2}$ cal degK^{-1}gfw^{-1} $298.15^oK \leq T \leq 2000^oK$

Structure

MoO_2 retains a solid structure to its disproportionation temperature.

Heat of Formation

Heat of formation by Mah.[1]

Heat Capacity and Entropy

Low-temperature data by King.[2] High-temperature data by King et al,[3] valid to 1800°K extrapolated to 2000°K.

Melting and Vaporization

MoO_2 disproportionates rather than melts.

Further details by Barriault et al.[4]

References

1. Mah, A. D., J. Phys. Chem. 61, 1572 (1957).
2. King, E. G., J. Am. Chem. Soc. 80, 1799 (1959).
3. King, E. G. et al, U. S. Bur. Mines, Rept. 5664 (1960).
4. Barriault, R. J. et al, ASD TR 61-260 (May 1962), Pt. 1.

TABLE 161

MOLYBDENUM DIOXIDE

IDEAL MOLECULAR GAS

MoO_2

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Mo from 0° to 2890°K, Liquid Mo from 2890° to 4965°K, Gaseous Mo from 4965° to 6000°K; Gaseous O_2, Gaseous MoO_2

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.670	0.297	0.297	INFINITE
298.15	10.663	63.874	63.874	0.000	-0.200	-2.596	1.903
300	10.683	63.940	63.874	0.020	-0.204	-2.611	1.902
400	11.624	67.151	64.306	1.138	-0.380	-3.386	1.850
500	12.256	69.817	65.149	2.334	-0.523	-4.118	1.800
600	12.677	72.091	66.121	3.582	-0.653	-4.826	1.758
700	12.962	74.068	67.118	4.865	-0.782	-5.513	1.721
800	13.162	75.813	68.098	6.172	-0.913	-6.179	1.688
900	13.307	77.372	69.044	7.496	-1.053	-6.829	1.658
1000	13.414	78.780	69.948	8.832	-1.205	-7.462	1.631
1100	13.496	80.062	70.810	10.178	-1.378	-8.081	1.605
1200	13.559	81.240	71.631	11.531	-1.573	-8.681	1.581
1300	13.609	82.327	72.412	12.889	-1.792	-9.265	1.558
1400	13.649	83.337	73.157	14.252	-2.033	-9.832	1.535
1500	13.682	84.280	73.867	15.619	-2.286	-10.379	1.512
1600	13.709	85.164	74.546	16.988	-2.574	-10.909	1.490
1700	13.731	85.995	75.195	18.360	-2.892	-11.422	1.468
1800	13.750	86.781	75.817	19.734	-3.241	-11.912	1.446
1900	13.767	87.525	76.414	21.110	-3.623	-12.384	1.424
2000	13.780	88.231	76.967	22.488	-4.040	-12.834	1.402
2100	13.792	88.904	77.539	23.866	-4.496	-13.264	1.380
2200	13.803	89.546	78.070	25.246	-4.990	-13.669	1.358
2300	13.812	90.160	78.583	26.627	-5.524	-14.053	1.335
2400	13.820	90.748	79.077	28.008	-6.102	-14.410	1.312
2500	13.827	91.312	79.556	29.391	-6.725	-14.745	1.289
2600	13.833	91.854	80.018	30.774	-7.394	-15.051	1.265
2700	13.839	92.376	80.466	32.157	-8.112	-15.333	1.241
2800	13.844	92.880	80.901	33.541	-8.875	-15.585	1.216
2890	13.848	93.317	81.271	34.788	-9.612	-15.762	1.192
2890	13.848	93.317	81.271	34.788	-16.262	15.762	1.192
2900	13.848	93.366	81.322	34.926	-16.319	-15.785	1.190
3000	13.852	93.835	81.732	36.311	-16.886	-15.759	1.148
3100	13.856	94.290	82.129	37.696	-17.458	-15.708	1.107
3200	13.859	94.729	82.516	39.082	-18.034	-15.648	1.069
3300	13.862	95.156	82.893	40.468	-18.613	-15.563	1.031
3400	13.865	95.570	83.260	41.855	-19.194	-15.463	0.994
3500	13.868	95.972	83.617	43.241	-19.[illegible]	-15.341	0.958
3600	13.870	96.363	83.966	44.628	-20.37[illegible]	-15.206	0.923
3700	13.872	96.743	84.306	46.015	-20.969	-15.052	0.889
3800	13.874	97.113	84.638	47.403	-21.566	-14.885	0.856
3900	13.876	97.473	84.963	48.790	-22.168	-14.703	0.824
4000	13.878	97.824	85.280	50.178	-22.722	-14.500	0.792
4100	13.879	98.167	85.590	51.566	-23.380	-14.289	0.762
4200	13.881	98.501	85.893	52.954	-23.992	-14.057	0.731
4300	13.882	98.828	86.190	54.342	-24.607	-13.807	0.702
4400	13.884	99.147	86.481	55.730	-25.227	-13.548	0.673
4500	13.885	99.459	86.766	57.119	-25.849	-13.280	0.645
4600	13.886	99.764	87.046	58.507	-26.477	-12.990	0.617
4700	13.887	100.063	87.319	59.896	-27.109	-12.690	0.590
4800	13.888	100.355	87.588	61.284	-27.748	-12.374	0.563
4900	13.889	100.642	87.851	62.673	-28.392	-12.044	0.537
4965	13.890	100.824	88.019	63.576	-28.816	-11.817	0.520
4965	13.890	100.824	88.019	63.576	-170.113	-11.817	0.520
5000	13.890	100.922	88.110	64.062	-170.426	-10.705	0.468
5100	13.890	101.198	88.364	65.451	-171.351	-7.502	0.321
5200	13.891	101.467	88.613	66.840	-172.313	-4.280	0.180
5300	13.892	101.732	88.858	68.229	-173.312	-1.039	0.043
5400	13.893	101.992	89.099	69.619	-174.349	2.225	-0.090
5500	13.893	102.246	89.336	71.008	-175.425	5.511	-0.219
5600	13.894	102.497	89.569	72.397	-176.543	8.803	-0.344
5700	13.895	102.743	89.798	73.787	-177.703	12.135	-0.465
5800	13.895	102.984	90.023	75.176	-178.911	15.480	-0.496
5900	13.896	103.222	90.245	76.567	-180.169	18.839	-0.698
6000	13.896	103.455	90.463	77.955	-181.484	22.236	-0.810

May 1962 CHW

MOLYBDENUM DIOXIDE (MoO_2) (IDEAL MOLECULAR GAS) gfw = 127.95

ΔH^o_{f0} = 0.297 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = -0.200 kcal gfw^{-1}

Point Group = C_{2v}

$S^o_{298.15}$ = 63.874 cal degK^{-1}gfw^{-1}

$H^o_{298.15} - H^o_0$ = 2.670 kcal gfw^{-1}

Vibrational Levels and Multiplicities

ω, cm^{-1}	ω, cm^{-1}
824 (1)	857 (1)
367 (1)	

Bond lengths and angles:

Mo-O distance = 1.73 A

O-Mo-O Angle = 107 deg

Product of moments of inertia: $I_A I_B I_C = 6.2826 \times 10^{-115} g^3 cm^6$, σ - 2

Heat of Formation

Average of calculations based on data by DeMaria *et al*[1] and by Burns *et al.*[2]

Heat Capacity and Entropy

Calculated on polyatomic gas-computer program using estimated spectroscopic constants.

Further details by Barriault *et al.*[3]

References

1. DeMaria, G. *et al*, J. Chem. Phys. 32, 1373 (1960).
2. Burns, R. *et al*, J. Chem. Phys. 32, 1363 (1960).
3. Barriault, R. *et al*, ASD TR 61-260 (May 1962), Pt. 1.

TABLE 162

MOLYBDENUM TRIOXIDE

CONDENSED PHASE

MoO_3

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Mo from 0° to 2890°K, Liquid Mo from 2890° to 4965°K, Gaseous Mo from 4965° to 6000°K; Gaseous O_2, Solid MoO_3 from 0° to 1070°K, Liquid MoO_3 from 1070° to 1500°K.

T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
	cal/°K gfw			Kcal/gfw			
0	0.000	0.000	INFINITE	-3.009	-176.905	-176.905	INFINITE
298.15	17.934	18.580	18.580	0.000	-178.100	-159.686	117.048
300	17.977	18.691	18.581	0.033	-178.098	-159.572	116.243
400	19.777	24.130	19.310	1.928	-177.851	-153.431	83.827
500	21.030	28.684	20.742	3.971	-177.513	-147.361	64.408
600	22.067	32.612	22.400	6.127	-177.113	-141.369	51.491
700	23.001	36.084	24.11.	6.381	-176.659	-135.447	42.286
800	23.882	39.213	25.805	10.726	-176.152	-129.593	35.401
900	24.731	42.076	27.457	13.157	-175.591	-123.807	30.063
1000	25.560	44.724	29.053	15.671	-174.979	-118.084	25.806
1070	26.133	46.473	30.136	17.481	-174.526	-114.123	23.309
1070	30.200	57.392	30.136	29.164	-162.843	-114.123	23.309
1100	30.200	58.227	30.891	30.070	-162.519	-112.756	22.401
1200	30.200	60.855	33.280	33.090	-161.471	-108.277	19.719
1300	30.200	63.272	35.495	36.110	-160.456	-103.887	17.464
1400	30.200	65.511	37.561	39.130	-159.47.	-99.576	15.544
1500	30.200	67.594	39.494	42.150	-158.508	-95.331	13.889

May 1962 CHW

MOLYBDENUM TRIOXIDE (MoO_3) (CONDENSED PHASE) gfw = 143.95

$\Delta H^o_{f298.15}$ = -178.100 kcal gfw^{-1} $S^o_{298.15}$ = 18.58 cal degK^{-1}gfw^{-1}

T_m = 1070°K ΔH_m = 11.683 kcal gfw^{-1}

$H^o_{298.15} - H^o_0$ = 3.009 kcal gfw^{-1}

$C^o_p = 17.97 + 7.80 \times 10^{-3}T - 2.10 \times 10^5 T^{-2}$ cal degK^{-1}gfw^{-1} 298.15°K $\leq$ T $\leq$ 1070°K

C^o_p = 30.2 cal degK^{-1} gfw^{-1} 1070°K $\leq$ T $\leq$ 1500°K

Structure

MoO_3 melts at 1070°K.

Heat of Formation

Based on Mah.[1]

Heat Capacity and Entropy

Low-temperature data from Kelley and King.[2] High-temperature data by King *et al.*[3]

Melting and Vaporization

The melting point is an average of four values.

Further details given by Barriault *et al.*[4]

Referen es

1. Mah, A. D., J. Phys. Chem. 61, 1572 (1957).
2. Kelley, K. and E. King, U. S. Bur. Mines, Bull. 592 (1961).
3. King, E. *et al*, U. S. Bur. Mines, Rept. 5664 (1960).
4. Barriault, R. *et al*, ASD TR 61-260 (May 1962), Pt. 1.

TABLE 163

MOLYBDENUM TRIOXIDE

IDEAL MOLECULAR GAS

MoO_3

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Mo from 0° to 2890°K, Liquid Mo from 2890° to 4965°K, Gaseous Mo from 4965° to 6000°K, Gaseous O_2, Gaseous MoO_3

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-3.227	-80.023	-80.023	INFINITE
298.15	14.498	66.653	66.653	0.000	-81.000	-76.919	56.381
300	14.533	66.742	66.653	0.027	-81.004	-76.894	56.014
400	16.105	71.153	67.244	1.564	-81.115	-75.504	41.252
500	17.147	74.867	68.407	3.230	-81.154	-74.094	32.385
600	17.838	78.059	69.756	4.982	-81.158	-72.682	26.473
700	18.308	80.846	71.145	6.790	-81.150	-71.271	22.251
800	18.637	83.313	72.515	8.639	-81.139	-69.861	19.084
900	18.876	85.523	73.840	10.515	-81.133	-68.451	16.621
1000	19.052	87.521	75.110	12.412	-81.138	-67.041	14.651
1100	19.186	89.344	76.322	14.324	-81.165	-65.629	13.039
1200	19.291	91.018	77.478	16.248	-81.213	-64.216	11.695
1300	19.374	92.565	78.580	18.181	-81.285	-62.798	10.557
1400	19.440	94.004	79.631	20.122	-81.380	-61.373	9.580
1500	19.494	95.347	80.634	22.069	-81.489	-59.940	8.733
1600	19.539	96.606	81.593	24.021	-81.[illegible]32	-58.496	7.990
1700	19.576	97.792	82.512	25.977	-81.[illegible]08	-57.049	7.334
1800	19.607	98.912	83.392	27.936	-82.016	-55.586	6.749
1900	19.634	99.973	84.237	29.898	-82.259	-54.110	6.224
2000	19.657	100.981	85.049	31.862	-82.540	-52.620	5.750
2100	19.677	101.940	85.831	33.829	-82.860	-51.116	5.319
2200	19.694	102.856	86.584	35.798	-83.221	-49.597	4.927
2300	19.709	103.732	87.311	37.768	-83.624	-48.059	4.566
2400	19.722	104.571	88.013	39.739	-84.072	-46.507	4.235
2500	19.734	105.376	88.691	41.712	-84.569	-44.930	3.928
2600	19.744	106.150	89.348	43.686	-85.113	-43.334	3.642
2700	19.753	106.8[illegible]6	89.984	45.661	-85.709	-41.715	3.376
2800	19.762	107.614	90.601	47.637	-86.353	-40.071	3.128
2890	19.768	108.239	91.140	49.415	-86.983	-38.576	2.917
2890	19.768	108.239	91.140	49.415	-93.633	-38.576	2.917
2900	19.769	108.308	91.200	49.613	-93.677	-38.384	2.893
3000	19.776	108.[illegible]78	91.781	51.590	-94.128	-36.468	2.657
3100	19.782	109.626	92.346	53.568	-94.586	-34.531	2.434
3200	19.787	110.255	92.896	55.547	-95.050	-32.598	2.226
3300	19.792	110.864	93.432	57.526	-95.[illegible]5	-30.634	2.029
3400	19.797	111.455	93.953	59.505	-95.9[illegible]	-28.665	1.843
3500	19.801	112.028	94.461	61.485	-96.4[illegible]	-26.670	1.665
3600	19.805	112.586	94.957	63.466	-96.962	-24.667	1.497
3700	19.809	113.129	95.441	65.446	-97.453	-22.655	1.338
3800	19.812	113.657	95.913	67.427	-97.949	-20.626	1.186
3900	19.815	114.172	96.375	69.409	-98.451	-18.584	1.041
4000	19.818	114.674	96.826	71.390	-98.958	-16.528	0.903
4100	19.821	115.163	97.267	73.372	-99.470	-14.461	0.771
4200	19.823	115.641	97.699	75.354	-99.988	-12.382	0.644
4300	19.825	116.107	98.122	77.337	-100.509	-10.281	0.523
4400	19.827	116.563	98.536	79.319	-101.04[illegible]	-8.180	0.406
4500	19.829	117.004	98.941	81.302	-101.573	-6.066	0.295
4600	19.831	117.444	99.339	83.285	-102.114	-3.933	0.187
4700	19.833	117.871	99.729	85.269	-10[illegible].662	-1.791	0.083
4800	19.835	118.289	100.111	87.252	-103.219	0.370	-0.017
4900	19.836	118.698	100.486	89.235	-103.786	2.533	-0.113
4965	19.837	118.958	100.725	90.525	-104.161	3.957	-0.174
4965	19.837	118.958	100.725	90.525	-245.458	3.957	-0.174
5000	19.838	119.098	100.854	91.219	-245.745	5.710	-0.250
5100	19.839	119.491	101.216	93.203	-246.600	10.746	-0.460
5200	19.840	119.876	101.571	95.187	-247.497	15.798	-0.664
5300	19.841	120.254	101.920	97.171	-248.438	20.871	-0.861
5400	19.843	120.625	102.263	99.155	-249.245	25.969	-1.051
5500	19.844	120.989	102.600	101.139	-250.458	31.086	-1.235
5600	19.845	121.347	102.937	103.124	-251.544	36.210	-1.413
5700	19.846	121.698	103.258	105.[illegible]	-252.686	41.371	-1.586
5800	19.847	122.043	103.579	107.093	-253.890	46.551	-1.754
5900	19.847	122.383	103.875	109.078	-255.163	51.737	-1.916
6000	19.848	122.716	104.206	111.063	-256.[illegible]	56.964	-2.075

May 1962 CHW

MOLYBDENUM TRIOXIDE (MoO_3) (IDEAL MOLECULAR GAS) gfw = 143.95

ΔH^o_{f0} = -80.023 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = -81.000 kcal gfw^{-1}

Point Group = D_{3h}

$S^o_{298.15}$ = 66.653 cal $degK^{-1} gfw^{-1}$

$H^o_{298.15} - H^o_0$ = 3.227 kcal gfw^{-1}

Vibrational Levels and Multiplicities

ω, cm^{-1}	ω, cm^{-1}
800 (1)	897 (2)
344 (1)	317 (2)

Bond lengths and angles:

Mo-O distance = 1.73 Å

O-Mo-O Angle = 120 deg

Product of moments of inertia: $I_A I_B I_C = 3.392032 \times 10^{-114} g^3 cm^6$, $\sigma = 6$

Heat of Formation

An average based on the works of DeMaria et al[1] and Burns et al.[2]

Heat Capacity and Entropy

Calculated on polyatomic gas-computer program using estimated spectroscopic constants.

Further details given by Barriault et al.[3]

References

1. DeMaria, G. et al, J. Chem. Phys. 32, 1373 (1960).
2. Burns, R. et al, J. Chem. Phys. 32, 1363 (1960).
3. Barriault, R. J. et al, ASD TR 61-260 (May 1962), Pt. 1.

NITROGEN IDEAL MONATOMIC GAS **N**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p:
Gaseous N_2 from 0° to 6000°K

T, °K	cal/°K gfw C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	Kcal/gfw $H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.481	112.536	112.536	INFINITE
298.15	4.968	36.615	36.615	0.000	112.980	108.887	-79.812
300	4.968	36.645	36.615	0.009	112.983	108.861	-79.301
400	4.968	38.074	36.809	0.506	113.131	107.465	-58.713
500	4.968	39.183	37.177	1.003	113.277	106.032	-46.344
600	4.968	40.089	37.590	1.500	113.417	104.569	-38.087
700	4.968	40.855	38.003	1.996	113.550	103.084	-32.183
800	4.968	41.518	38.402	2.493	113.675	101.580	-27.749
900	4.968	42.103	38.781	2.990	113.792	100.061	-24.297
1000	4.968	42.627	39.140	3.487	113.902	98.530	-21.533
1100	4.968	43.100	39.479	3.984	114.005	96.987	-19.269
1200	4.968	43.533	39.799	4.481	114.101	95.437	-17.381
1300	4.968	43.930	40.101	4.977	114.192	93.879	-15.782
1400	4.968	44.298	40.388	5.474	114.278	92.312	-14.410
1500	4.968	44.641	40.661	5.971	114.361	90.740	-13.220
1600	4.968	44.962	40.919	6.468	114.440	89.164	-12.179
1700	4.968	45.263	41.166	6.965	114.516	87.580	-11.259
1800	4.968	45.547	41.402	7.461	[illegible]	85.993	-10.440
1900	4.969	45.816	41.627	7.958	114.658	84.402	-9.708
2000	4.969	46.070	41.843	8.455	114.726	82.810	-9.049
2100	4.970	46.313	42.050	8.952	114.792	81.211	-8.451
2200	4.971	46.544	42.249	9.449	114.857	79.610	-7.908
2300	4.972	46.765	42.441	9.946	114.920	78.006	-7.412
2400	4.975	46.977	42.625	10.444	114.982	79.402	-6.957
2500	4.978	47.180	42.803	10.941	115.042	74.792	-6.538
2600	4.982	47.375	42.976	11.439	115.102	73.179	-6.151
2700	4.987	47.563	43.142	11.938	115.162	71.567	-5.793
2800	4.993	47.745	43.303	12.437	115.221	69.952	-5.460
2900	5.001	47.920	43.459	12.936	115.278	68.334	-5.150
3000	5.010	48.090	43.611	13.437	115.337	66.714	-4.860
3100	5.022	48.254	43.758	13.938	115.397	65.091	-4.589
3200	5.035	48.414	43.901	14.441	115.455	63.469	-4.335
3300	5.050	48.569	44.040	14.945	115.515	61.843	-4.095
3400	5.066	48.720	44.176	15.451	115.575	60.215	-3.870
3500	5.085	48.867	44.308	15.959	115.638	58.584	-3.658
3600	5.107	49.011	44.436	[illegible]	[illegible]	56.956	-3.458
3700	5.130	49.151	44.562	16.980	[illegible]	55.323	-3.268
3800	5.155	49.288	44.684	17.494	115.83	53.691	-3.088
3900	5.183	49.422	44.804	18.011	115.902	52.054	-2.917
4000	5.213	49.554	44.921	18.531	115.973	50.416	-2.754
4100	5.244	49.683	45.036	19.054	116.048	48.774	-2.600
4200	5.278	49.810	45.148	19.590	116.124	47.137	-2.452
4300	5.314	49.935	45.258	20.110	116.205	45.487	-2.312
4400	5.351	50.057	45.366	20.643	116.287	43.843	-2.178
4500	5.390	50.178	45.471	21.180	116.374	42.195	-2.049
4600	5.431	50.297	45.575	21.721	116.465	40.544	-1.926
4700	5.473	50.414	45.676	22.266	116.558	38.899	-1.809
4800	5.517	50.530	45.776	22.816	116.656	37.246	-1.696
4900	5.562	50.644	45.875	23.369	116.758	35.584	-1.587
5000	5.608	50.757	45.971	[illegible]	[illegible]	33.930	-1.483
5100	5.654	50.686	46.066	24.491	116.974	[illegible]	-1.383
5200	5.702	50.978	46.159	25.059	117.089	[illegible]	-1.286
5300	5.751	51.088	46.251	[illegible]	117.208	28.948	-1.194
5400	5.800	51.195	46.342	26.709	117.332	27.277	-1.104
5500	5.850	51.302	46.431	26.792	117.460	25.612	-1.018
5600	5.899	51.408	46.519	27.379	117.592	23.940	-0.934
5700	5.950	51.513	46.606	27.971	117.730	22.266	-0.854
5800	6.000	51.617	46.691	28.569	117.872	20.592	-0.776
5900	6.050	51.720	46.776	29.171	118.019	18.910	-0.700
6000	6.100	51.822	46.859	29.779	118.170	17.226	-0.627

May 1962 RCF

NITROGEN, MONATOMIC (N) (IDEAL GAS) gfw = 14.008

ΔH^o_{f0} = 112.536 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 112.980 kcal gfw^{-1}

Ground State Configuration $^4S_{1\text{-}1/2}$

$S^o_{298.15}$ = 36.615 cal deg K^{-1} gfw^{-1}

$H^o_{298.15} - H^o_0$ = 1.481 kcal gfw^{-1}

Electronic Levels and Multiplicities

Atomic energy levels from Moore.[1]

Heat of Formation

Based on review by Brewer and Searcy.[2]

Heat Capacity and Entropy

Calculated on monatomic gas-computer program.

Further details in report by Barriault *et al.*[3]

References

1. Moore, C. Atomic Energy Levels, Vol. 1, Nat. Bur. Stds. (1949).
2. Brewer, L. and A. Searcy, Ann. Rev. Phys. Chem. 8, 259 (1956).
3. Barriault, R. *et al*, ASD TR 61-260 (May 1962), Pt. I.

NITROGEN, MONATOMIC (N) (IDEAL GAS) GFW = 14.008

SUMMARY OF UNCERTAINTY ESTIMATES

T °K	C_p (cal °K gfw)	S_T (cal °K gfw)	$-(F_T - H_{298})/T$ (cal °K gfw)	$H_T - H_{298}$ (kcal gfw)	ΔH_f (kcal gfw)	ΔF_f (kcal gfw)	Log K_p
298.15	±0.000	±0.002	±0.002	±0.000	±0.100	±0.100	0.070
1000	±0.000	±0.002	±0.002	±0.000	±0.100	±0.100	0.020
2000	±0.000	±0.002	±0.002	±0.000	±0.100	±0.110	0.010
3000	±0.000	±0.002	±0.002	±0.001	±0.100	±0.110	0.010
4000	±0.000	±0.002	±0.002	±0.001	±0.100	±0.120	0.005
5000	±0.001	±0.002	±0.002	±0.001	±0.100	±0.120	0.005
6000	±0.001	±0.002	±0.003	±0.002	±0.100	±0.130	0.005

TABLE 165

NIOBIUM NITRIDE — CONDENSED PHASE — **NNb**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p. Solid Nb from 0° to 2741°K, Liquid Nb from 2741° to 5031°K, Gaseous Nb from 5031° to 6000°K; Gaseous N_2, Solid NbN from 0° to 2323°K, Liquid NbN from 2323° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.846	-56.046	-56.046	INFINITE
298.15	10.300	10.500	10.500	0.000	-56.500	-50.124	36.740
300	10.310	10.564	10.500	0.019	-56.498	-50.084	36.485
400	10.850	13.604	10.911	1.077	-56.389	-47.961	26.204
500	11.390	16.083	11.705	2.189	-56.237	-45.872	20.050
600	11.930	18.207	12.615	3.355	-56.047	-43.815	15.959
600	11.930	18.207	12.615	3.355	-56.047	-43.815	15.959
700	12.128	20.061	13.550	4.558	-55.835	-41.794	13.048
800	12.327	21.694	14.468	5.781	-55.622	-39.803	10.873
900	12.525	23.157	15.353	7.023	-55.408	-37.838	9.188
1000	12.724	24.487	16.201	8.286	-55.189	-35.898	7.845
1100	12.922	25.709	17.011	9.568	-54.968	-33.979	6.751
1200	13.121	26.842	17.783	10.870	-54.742	-32.081	5.842
1300	13.319	27.900	18.521	12.192	-54.512	-30.202	5.077
1400	13.518	28.894	19.227	13.534	-54.276	-28.340	4.424
1500	13.716	29.834	19.903	14.896	-54.034	-26.496	3.860
1600	13.915	30.725	20.552	16.277	-53.786	-24.669	3.369
1643	14.000	31.095	20.823	16.877	-53.676	-23.888	3.177
1643	15.000	31.704	20.823	17.877	-52.676	-23.888	3.177
1700	[illegible]	32.215	21.196	18.732	-52.476	-22.893	2.943
1800	15.000	33.073	21.833	20.232	-52.134	-21.163	2.569
1900	15.000	33.884	22.446	21.732	-51.805	-19.451	2.237
2000	15.000	34.653	23.[illegible]37	23.232	-51.487	-17.755	1.940
2100	15.000	35.385	23.608	24.732	-51.180	-16.077	1.673
2200	15.000	36.063	24.15[illegible]	26.232	-50.885	-17.713	1.760
2300	15.000	36.750	24.6[illegible]	27.732	-50.601	-12.760	1.212
2323	15.000	36.89[illegible]	24.812	28.0[illegible]7	-50.537	-12.073	1.136
2323	15.000	41.634	24.81[illegible]	39.077	-39.537	-12.073	1.136
2400	15.000	42.123	25.360	40.232	-39.129	-11.488	1.046
2500	15.000	42.736	26.043	41.732	-39.067	-10.331	0.903
2600	15.000	43.324	26.696	43.232	-38.816	-9.187	0.772
2700	15.000	43.84[illegible]	27.322	44.732	-38.575	-8.051	0.652
2741	15.000	44.116	27.572	45.347	-38.480	-7.591	0.605
2741	15.000	44.116	27.572	45.347	-44.880	-7.591	0.605
2800	15.000	44.436	27.9[illegible]4	46.[illegible]	-44.726	6.789	0.530
2900	15.000	44.762	28.[illegible]	47.732	-44.468	[illegible].435	0.410
3000	15.000	45.470	29.260	49.2[illegible]	-44.210	[illegible].099	0.299
3100	15.000	45.962	29.[illegible]	50.732	-43.952	-2.763	0.195
3200	15.000	46.43[illegible]	30.16[illegible]	52.232	-43.696	-1.441	0.098
3300	15.000	46.900	30.618	53.732	-43.440	-0.124	0.008
3400	15.000	47.346	31.103	55.232	-43.185	1.188	-0.076
3500	15.000	47.783	31.573	56.732	-42.931	2.489	-0.155
3600	15.000	48.20[illegible]	32.[illegible]	58.232	-42.677	3.778	-0.229
3700	15.000	48.616	32.47[illegible]	59.732	-42.424	5.068	-0.299
3800	15.000	49.016	32.[illegible]	61.232	-42.171	6.346	-0.365
3900	15.000	49.40[illegible]	33.321	62.732	-41.919	7.[illegible]20	-0.427
4000	15.000	49.78[illegible]	33.728	64.232	-41.668	8.888	-0.486
4100	15.000	50.156	34.124	65.732	-41.41[illegible]	10.150	-0.541
4200	15.000	50.518	34.510	67.232	-41.166	11.49[illegible]	-0.593
4300	15.000	50.871	34.886	68.732	-40.915	12.65[illegible]	-0.643
4400	15.000	51.215	35.253	70.[illegible]	-40.666	13.90[illegible]	-0.690
4500	15.000	51.[illegible]	35.612	71.[illegible]	-40.416	15.133	-0.735
4600	15.000	51.882	35.962	73.232	-40.167	16.366	-0.778
4700	15.000	52.205	36.304	74.732	-39.918	17.591	-0.818
4800	15.000	52.521	36.639	76.232	-39.670	18.812	-0.856
4900	15.000	52.830	36.966	77.732	-39.422	20.031	-0.893
5000	15.000	53.133	37.286	79.[illegible]32	-39.175	[illegible]1.240	-0.928
5031.58	15.000	53.227	37.386	79.706	-39.097	21.555	-0.936
5031.58	15.000	53.227	37.386	79.706	-201.670	21.555	-0.936
5100	15.000	[illegible].430	37.6[illegible]	80.732	-[illegible].542	24.5[illegible]	-1.054
5200	15.000	53.721	37.9[illegible]	82.[illegible]32	-[illegible].362	29.010	-1.220
5300	15.000	54.007	38.[illegible]8	83.732	-[illegible]01.188	33.457	-1.380
5400	15.000	54.287	38.503	85.232	-201.019	37.884	-1.533
5500	15.000	54.563	38.793	86.732	-200.856	42.299	-1.681
5600	15.000	54.833	39.[illegible]77	88.232	-200.698	46.719	-1.823
5700	15.000	55.098	39.356	89.732	-200.545	51.133	-1.960
5800	15.000	55.359	39.629	91.232	-200.396	55.556	-2.093
5900	15.000	55.616	39.898	92.732	-200.252	59.966	-2.221
6000	15.000	55.868	40.162	94.232	-200.112	64.373	-2.345

31 December 1963 HLS

NIOBIUM NITRIDE (NbN) (CONDENSED PHASE) gfw = 106.918

$\Delta H^{o}_{f298.15}$ = -56.5 kcal gfw^{-1}

$S^{o}_{298.15}$ = 10.5 cal degK^{-1}gfw^{-1}

T_t = 1643°K

ΔH_t = 1.0 kcal gfw^{-1}

T_m = 2323°K

ΔH_m = 11.0 kcal gfw^{-1}

$H^{o}_{298.15}-H^{o}_{0}$ = 1.846 kcal gfw^{-1}

C^{o}_{p} = 8.69 + 5.40 x 10^{-3}T cal degK^{-1}gfw^{-1} 298.15°K ≤ T ≤ 600°K

C^{o}_{p} = 10.7391 + 1.9847 x 10^{-3}T cal degK^{-1}gfw^{-1} 600°K ≤ T ≤ 1643°K

C^{o}_{p} = 15.0 cal degK^{-1}gfw^{-1} 1643°K ≤ T ≤ 6000°K

Structure

Low-temperature form is hcp. Above 1643°K, it is consider to be fcc.

Heat of Formation

Based on combustion data of Mah and Gellert.[1]

Heat Capacity and Entropy

Low-temperature data estimated. Data from 298.15° to 600°K based on Kelley.[2] Data above 600°K estimated.

Melting and Vaporization

Heats of transition and melting estimated.

References

1. Mah, A. D. and N. L. Gellert, J. Am. Chem. Soc. 78, 3261 (1956).

2. K. K. Kelley, U. S. Bur. Mines, Bull. 584 (1960).

NIOBIUM NITRIDE (NbN) (CONDENSED PHASE) GFW = 106.918

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^{o}_{p} (cal/°K gfw)	S^{o}_{T} (cal/°K gfw)	$-(F^{o}_{T} - H^{o}_{298})/T$ (cal/°K gfw)	$H^{o}_{T} - H^{o}_{298}$ (Kcal/gfw)	ΔH^{o}_{f} (Kcal/gfw)	ΔF^{o}_{f} (Kcal/gfw)	Log K_p
298.15	± 0.500	± 1.000	± 1.000	± 0.000	±0.400		
600	± 0.500	± 1.350	± 1.098	± 0.151			
600	± 1.000	± 1.350	± 1.098	± 0.151			
1000	± 1.000	± 1.860	± 1.310	± 0.551			
1643	± 1.000	± 2.357	± 1.630	± 1.194			
1643	± 2.000	± 2.966	± 1.630	± 2.194			
2000	± 2.000	± 3.359	± 1.905	± 2.908			
2323	± 2.000	± 3.658	± 2.128	± 3.554			
2323	± 2.000	± 5.380	± 2.128	± 7.554			
3000	± 2.000	± 5.892	± 2.922	± 8.908			
4000	± 2.000	± 6.467	± 3.740	±10.908			
5000	± 2.000	± 6.913	± 4.332	±12.908			
6000	± 2.000	± 7.278	± 4.793	±14.908			

TABLE 166

DINIOBIUM NITRIDE CONDENSED PHASE **NNb_2**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Nb from 0° to 2741°K, Liquid Nb from 2741° to 5031°K, Gaseous Nb from 5031° to 6000°K; Gaseous N_2, Solid Nb_2N from 0° to 2673°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.938	-59.874	-59.874	INFINITE
298.1'	16.130	19.000	19.000	0.000	-60.500	-53.975	39.563
300	16.138	19.100	19.000	0.030	-60.498	-53.934	39.289
400	16.547	23.798	19.638	1.664	-60.413	-51.756	28.278
500	16.955	27.534	20.856	3.339	-60.307	-49.608	21.682
600	17.364	30.662	22.237	5.055	-60.186	-47.478	17.293
700	17.773	33.369	23.638	6.812	-60.048	-45.372	14.165
800	18.182	35.769	25.067	8.610	-59.898	-43.284	11.824
900	18.591	37.935	26.325	10.448	-59.736	-41.218	10.009
1000	19.000	39.914	27.586	12.328	-59.557	-39.170	8.560
1000	19.000	39.914	27.586	12.328	-59.557	-39.170	8.560
1100	19.209	41.735	28.791	14.238	-59.375	-37.139	7.378
1200	19.418	43.416	29.941	16.170	-59.195	-35.127	6.397
1300	19.628	44.978	31.038	18.122	-59.021	-33.128	5.569
1400	19.837	46.440	32.087	20.095	-58.851	-31.141	4.861
1500	20.046	47.816	33.090	22.090	-58.680	-29.169	4.250
1600	20.255	49.117	34.051	24.105	-58.51[illegible]	-27.206	3.716
1700	20.464	50.351	34.974	26.141	-58.3[illegible]	-25.257	3.247
1800	20.674	51.526	35.861	28.197	-58.182	-23.315	2.831
1900	20.883	52.650	36.715	30.275	-58.019	-21.380	2.459
2000	21.092	53.726	37.539	32.374	-57.855	-19.455	2.126
2100	21.301	54.760	38.335	34.494	-57.691	-17.540	1.825
2200	21.510	55.756	39.104	36.634	-57.528	-18.934	1.881
2300	21.720	56.717	39.849	38.796	-57.365	-13.731	1.305
2400	21.929	57.646	40.571	40.978	-57.202	-11.840	1.078
2500	22.138	58.545	41.273	43.182	-57.037	-9.951	0.870
2600	22.347	59.417	41.954	45.406	-56.873	-8.072	0.679
2673	22.[illegible]	60.038	42.439	47.043	-56.753	-6.701	0.548

31 December 1963 HLS

TANTALUM NITRIDE (TaN) (CONDENSED PHASE) gfw 194.958

$\Delta H^o_{f298.15}$ = -59.95 kcal gfw^{-1} $S^o_{298.15}$ 12.0 cal degK^{-1}gfw^{-1}

T_m = 3363°K ΔH_m = 16.0 kcal gfw^{-1}

$H^o_{298.15}-H^o_0$=1.779 kcal gfw^{-1}

C^o_p = 7.73 + 7.80 x 10^{-3}T cal degK^{-1}gfw^{-1} 298.15°K ≤ T ≤ 1000°K

C^o_p = 15.53 cal deg K^{-1}gfw^{-1} 1000°K ≤ T ≤ 3363°K

C^o_p = 15.0 cal deg K^{-1} gfw^{-1} 3363°K ≤ T ≤ 6000°K

Structure

TaN has an hexagonal structure and a limited homogeneity range.

Heat of Formation

Data of Mah and Gellert[1] slightly altered.

Heat-Capacity and Entropy

Low-temperature data estimated. Data from 298.15° to 1000°K use Kelley[2] equation which is extrapolated above 773°K. Data above 1000°K estimated.

Melting and Vaporization

Heat of melting estimated.

References

1. Mah, A. D. and N. L. Gellert, J. Am. Chem. Soc 78, 3261 (1956).

2. Kelley, K. K., U. S. Bur. Mines, Bull. 584 (1960).

TANTALUM NITRIDE (TaN) (CONDENSED PHASE) GFW = 194.958

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal °K gfw)	S^o_T (cal °K gfw)	$-(F^o_T - H^o_{298})/T$ (cal °K gfw)	$H^o_T - H^o_{298}$ (Kcal gfw)	ΔH_f (Kcal gfw)	ΔF_f (Kcal gfw)	Log K_p
298.15	± 0.200	± 1.000	± 1.000	± 0.000	± 4.000		
1000	± 0.200	± 1.242	± 1.102	± 0.140			
1000	± 1.000	± 1.242	± 1.102	± 0.140			
2000	± 1.000	± 1.935	± 1.365	± 1.140			
2000	± 2.000	± 1.935	± 1.365	± 1.140			
3000	± 2.000	± 2.746	± 1.699	± 3.140			
3363	± 2.000	± 2.975	± 1.825	± 3.866			
3363	± 2.000	± 4.461	± 1.825	± 8.866			
4000	± 2.000	± 4.808	± 2.273	±10.140			
5000	± 2.000	± 5.255	± 2.826	±12.140			
6000	± 2.000	± 5.619	± 3.262	±14.140			

DITANTALUM NITRIDE CONDENSED PHASE NTa_2

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ta from 0° to 3270°K, Liquid Ta from 3270° to 5706°K, Gaseous Ta from 5706° to 6000°K, Gaseous N_2, Solid Ta_2N from 0° to 3000°K, Liquid Ta_2N from 3000° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-3.163	-64.011	-64.011	INFINITE
298.15	16.205	22.000	22.000	0.000	-64.600	-58.421	42.821
300	16.237	22.100	22.000	0.030	-64.598	-58.382	42.529
400	17.478	26.958	22.654	1.722	-64.493	-56.324	30.772
500	18.280	30.949	23.926	3.51[illegible]	-64.320	-54.300	23.734
600	18.908	34.339	[illegible].386	5.372	-64.101	-52.317	19.055
700	19.454	37.24[illegible]	26.88[illegible]	7.291	-63.843	-50.372	15.726
800	19.957	39.927	28.250	9.261	-63.557	-48.467	13.240
900	20.434	42.30[illegible]	29.77[illegible]	11.281	-63.237	-46.599	11.315
1000	20.896	44.482	31.134	13.348	-62.889	-44.770	9.784
1100	21.347	46.495	32.440	15.460	-62.509	-42.976	8.538
1200	21.791	48.371	33.691	17.617	-62.102	-41.219	7.507
1300	22.230	50.13[illegible]	34.888	19.818	-61.665	-39.495	6.639
1400	22.666	51.79[illegible]	36.037	22.063	-61.200	-37.806	5.902
1500	23.099	53.375	37.141	24.351	-60.713	-36.153	5.267
1600	23.530	54.87[illegible]	38.20[illegible]	26.683	-60.197	-34.532	4.717
1700	23.959	56.315	39.226	29.057	-59.[illegible]	-32.944	4.235
1800	24.388	57.700	40.215	31.474	-59.0[illegible]	-31.389	3.811
1900	24.815	59.030	41.170	33.934	-58.506	-29.867	3.435
2000	25.241	60.314	42.095	36.437	-57.957	-28.375	3.101
2100	[illegible]	[illegible]	[illegible]	38.983	-57.278	-26.915	2.801
2200	[illegible]	[illegible]	[illegible]	41.571	-56.639	-28.781	2.859
2300	26.518	[illegible]	44.[illegible]	44.201	-55.991	-24.077	2.288
2400	[illegible]	[illegible]	[illegible]	46.874	-55.3[illegible]	-22.710	2.068
2500	[illegible]	66.17[illegible]	45.3[illegible]	49.590	-54.683	-21.361	1.867
2600	[illegible]	[illegible]	[illegible]	52.347	-54.030	-20.043	1.685
2700	[illegible]	[illegible]	47.888	55.146	-53.402	-18.743	1.517
2800	[illegible]	[illegible]	[illegible]	57.[illegible]	-52.814	-17.476	1.364
2900	[illegible]	70.[illegible]	[illegible]	60.875	-52.[illegible]	-16.221	1.222
3000	[illegible]	71.[illegible]	[illegible]	63.80[illegible]	-51.842	-14.989	1.092
3000	[illegible]	76.685	[illegible]	85.80	-29.842	-14.989	1.092
3100	[illegible]	79.42[illegible]	[illegible]	88.05[illegible]	-30.[illegible]	-14.487	1.021
3200	[illegible]	[illegible]	[illegible]	[illegible]	-30.[illegible]	-13.974	0.754
3270	[illegible]	[illegible]	[illegible]	91.[illegible]	-31.204	-13.598	0.909
3270	[illegible]	[illegible]	[illegible]	91.877	-44.[illegible]	-13.598	0.909
3300	[illegible]	[illegible]	[illegible]	[illegible]	-44.[illegible]	-13.3[illegible]	0.882
3400	[illegible]	81.[illegible]	[illegible]	94.80[illegible]	-44.467	-12.37[illegible]	0.795
3500	[illegible]	[illegible]	[illegible]	[illegible]	-44.3[illegible]	11.424	0.713
3600	[illegible]	[illegible]	[illegible]	[illegible].30[illegible]	-44.260	-10.488	0.637
3700	[illegible]	[illegible]	[illegible]	101.[illegible]	-44.1[illegible]	-9.551	0.564
3800	[illegible]	[illegible]	56.[illegible]	10[illegible]	-44.053	-8.617	0.496
3900	[illegible]	[illegible]	[illegible]	106.[illegible]	-43.951	-7.687	0.431
4000	[illegible]	[illegible]	[illegible]	108.30[illegible]	-43.850	-6.760	0.369
4100	22.[illegible]	[illegible]	[illegible]	110.55[illegible]	-43.748	-5.835	0.311
4200	[illegible]	[illegible]	[illegible]	112.80[illegible]	-43.647	-4.907	0.255
4300	[illegible]	[illegible]	60.[illegible]	115.052	-43.547	-3.989	0.203
4400	[illegible]	87.[illegible]	[illegible]	117.30[illegible]	-43.447	-3.070	0.153
4500	[illegible]	[illegible]	[illegible]	119.552	-43.348	-2.156	0.105
4600	22.[illegible]	[illegible]	61.824	121.80[illegible]	-43.24[illegible]	-1.237	0.059
4700	22.[illegible]	88.786	[illegible]	124.052	-43.150	-0.323	0.015
4800	[illegible]	89.[illegible]	62.947	126.30[illegible]	-43.052	0.589	-0.027
4900	[illegible]	[illegible]	63.489	128.55[illegible]	-42.954	1.[illegible]89	-0.066
5000	22.[illegible]	90.[illegible]	[illegible]	[illegible]	-42.857	[illegible].395	-0.105
5100	22.500	90.624	64.535	133.05[illegible]	-42.759	3.309	-0.142
5200	22.500	91.061	[illegible]	[illegible]	-42.663	4.206	-0.177
5300	22.500	91.4[illegible]	[illegible]	[illegible]	-42.566	5.106	-0.211
5400	22.500	91.910	66.[illegible]	139.80[illegible]	-42.470	6.002	-0.243
5500	22.50[illegible]	[illegible]	66.495	142.05[illegible]	-42.374	6.903	-0.274
5600	22.500	[illegible]	66.96[illegible]	144.30[illegible]	-42.279	7.802	-0.304
5700	22.500	93.12[illegible]	67.[illegible]	14[illegible]	-42.186	8.685	-0.333
5706.6[illegible]	22.50[illegible]	[illegible]	67.44[illegible]	146.7[illegible]	-42.176	8.742	-0.335
5706.6[illegible]	22.50[illegible]	[illegible]	67.446	146.7[illegible]	404.62[illegible]	8.742	-0.335
5800	22.5[illegible]	[illegible]	67.86[illegible]	148.80[illegible]	404.841	15.504	-0.584
5900	22.500	[illegible]	66.301	151.[illegible]	-405.083	22.749	-0.843
6000	22.5[illegible]	[illegible]	[illegible]	[illegible]	-405.331	30.011	-1.093

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DITANTALUM NITRIDE(Ta_2N) (CONDENSED PHASE) gfw = 375.908

$\Delta H^o_{f\,298.15}$ = -64.6 kcal gfw^{-1} $S^o_{298.15}$ = 22.0 cal degK^{-1}gfw^{-1}

T_m = 3000°K ΔH_m = 22.0 kcal gfw^{-1}

$H^o_{298.15} - H^o_0$ = 3.163 kcal gfw^{-1}

$C^o_p = 16.845 + 0.0042193T - 1.6868\times10^5 T^{-2}$ cal degK^{-1}gfw^{-1} 298.15°K ≤ T ≤ 3000°K

C^o_p = 22.5 cal degK^{-1}gfw^{-1} 3000°K ≤ T ≤ 6000°K

Structure

Ta_2N has an hexagonal structure and a variable homogeneity range.

Heat of Formation

Calorimetric value of Mah[1] used.

Heat Capacity and Entropy

Low-temperature data estimated. High-temperature data reported by Pears et al[2] recomputed assuming Ta_2N rather than TaN. See volume 1, this work (section IVB27.3.2) for details.

Melting and Vaporization

Heat of fusion estimated.

References

1. Mah, A. D., J. Am. Chem. Soc. 80, 3872 (1958).

2. Pears, C. D., et al, ASD TDR 62-765 (January 1963).

DITANTALUM NITRIDE (Ta_2N) (CONDENSED PHASE) GFW = 375.908

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T (cal/°K gfw)	$-(F_T - H_{298})/T$ (cal/°K gfw)	$H_T - H_{298}$ (kcal gfw)	ΔH_f (kcal gfw)	ΔF_f (kcal gfw)	Log K_p
298.15	± 1.000	± 2.000	± 2.000	± 0.000			
1000	± 1.000	± 3.210	± 2.508	± 0.702			
1000	± 2.000	± 3.210	± 2.508	± 0.702			
2000	± 2.000	± 4.596	± 3.246	± 2.702			
3000	± 2.000	± 5.407	± 3.840	± 4.702			
3000	± 3.000	± 7.074	± 3.840	± 9.702			
4000	± 3.000	± 7.937	± 4.762	± 12.702			
5000	± 3.000	± 8.607	± 5.466	± 15.702			
6000	± 3.000	± 9.153	± 6.037	± 18.702			

TITANIUM NITRIDE

CONDENSED PHASE

NTi

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ti from 0° to 1950°K, Liquid Ti from 1950° to 3550°K, Gaseous Ti from 3550° to 6000°K, Gaseous N_2, Solid TiN from 0° to 3223°K, Liquid TiN from 3223° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.310	-79.874	-79.874	INFINITE
298.15	8.860	7.240	7.240	0.000	-80.750	-73.900	54.167
300	8.903	7.295	7.240	0.016	-80.751	-73.857	53.802
400	10.436	10.096	7.612	0.994	-80.742	-71.558	39.095
500	11.196	12.514	8.357	2.079	-80.657	-69.270	30.277
600	11.652	[illegible]	9.221	3.223	-80.543	-67.003	24.405
700	11.964	16.420	10.128	4.405	-80.418	-64.757	20.217
800	12.199	18.033	11.01	5.613	-80.292	-62.528	17.081
900	12.391	19.457	11.878	6.843	-80.167	-60.314	14.646
1000	12.554	20.796	12.705	8.090	-80.047	-58.115	12.700
1100	12.699	21.999	13.496	9.353	-79.932	-55.928	11.111
1155	12.774	22.621	13.916	10.054	-79.870	-54.728	10.355
1155	12.774	22.621	13.916	10.054	-80.820	-54.728	10.355
1200	12.832	23.110	[illegible]	10.640	-80.771	-53.713	9.782
1300	12.957	24.142	14.773	11.919	-80.666	-51.463	8.651
1400	13.075	25.107	15.663	13.221	-80.564	-49.220	7.683
1500	13.188	26.011	16.324	14.534	-80.466	-46.986	6.845
1600	13.298	26.867	16.956	15.859	-80.370	-44.757	6.113
1700	13.406	27.677	17.563	17.194	-80.277	-42.534	5.468
1800	13.511	28.446	18.146	18.540	-80.186	-40.316	4.895
1900	13.614	29.179	18.708	19.896	-80.098	-38.104	4.383
1950	[illegible]	[illegible]	18.981	20.578	-80.054	-36.999	4.147
1950	13.665	29.534	18.981	20.578	-83.754	-36.999	4.147
2000	13.716	29.860	19.243	21.262	-83.686	-35.891	3.912
2100	13.817	[illegible]	19.771	22.639	-83.539	-33.410	3.477
2200	13.917	31.137	20.276	24.026	-83.385	-34.327	3.410
2300	14.016	31.818	20.764	25.422	-83.222	-28.649	2.722
2400	14.115	[illegible]	21.238	26.829	-8 .052	-26.282	2.393
2500	14.213	[illegible]	21.696	28.245	-82.873	-23.919	2.091
2600	14.310	33.556	22.142	29.672	-82.684	-21.565	1.813
2700	14.407	34.096	22.574	31.107	-82.488	-19.217	1.555
2800	14.504	34.621	22.995	32.553	-82.292	-16.876	1.317
2900	14.601	35.132	23.405	34.008	-82.069	-14.544	1.096
3000	14.697	[illegible]	23.804	35.473	-81.846	-12.221	0.890
3100	14.793	36.117	24.194	36.948	-81.614	-9.907	0.698
3200	14.889	36.563	24.573	.432	-81.374	-7.595	0.519
3223	14.911	36.690	24.660	38.774	-81.317	-7.066	0.479
3223	16.000	41.344	24.660	53.774	-66.317	-7.066	0.479
3300	16.000	41.722	25.053	[illegible]	-66.043	-5.650	0.374
3400	16.000	42.200	25.551	56.606	-65.688	-3.828	0.246
3500	16.000	42.663	26.033	58.206	-65.344	-2.014	0.126
3550	16.000	42.890	26.269	59.006	-65.157	-1.113	0.069
3550	16.000	42.890	26.269	59.006	-167.614	-1.113	0.069
3600	16.000	43.114	26.501	59.806	-167.442	1.233	-0.075
3700	16.000	43.552	26.956	61.406	-167.109	5.915	-0.349
3800	16.000	43.971	27.399	63.006	-166.790	10.585	-0.609
3900	16.000	44.376	27.829	64.606	-166.486	15.248	-0.854
4000	16.000	44.100	28.248	66.206	-166.194	19.906	-1.088
4100	16.000	45.195	28.657	67.806	-165.916	24.554	-1.309
4200	16.000	45.580	29.055	69.406	[illegible]	29.200	-1.519
4300	16.000	45.957	29.444	71.006	-165.397	33.834	-1.720
4400	16.000	46.325	29.823	72.606	-165.155	[illegible]	-1.911
4500	16.000	46.686	30.194	74.206	-164.925	[illegible]	-2.093
4600	16.000	47.036	30.556	75.806	-164.705	47.712	-2.267
4700	16.000	47.380	30.911	77.406	-164.496	52.321	-2.433
4800	16.000	47.717	31.257	79.006	-164.297	56.938	-2.592
4900	16.000	48.047	31.597	80.606	-164.107	61.544	-2.745
5000	16.000	48.370	31.929	82.206	-163.925	66.145	-2.891
5100	16.000	48.687	32.254	83.806	-163.753	70.748	-3.032
5200	16.000	48.998	32.573	85.406	-163.588	75.344	-3.166
5300	16.000	49.302	32.886	87.006	-163.431	79.941	-3.296
5400	16.000	49.602	33.193	88.606	-163.281	84.525	-3.421
5500	16.000	49.895	33.494	90.206	-163.137	89.115	-3.541
5600	16.000	50.183	33.789	91.806	-163.000	93.701	-3.657
5700	16.000	50.467	34.080	93.406	-162.868	98.281	-3.768
5800	16.000	50.745	34.364	95.006	-162.741	102.866	-3.876
5900	16.000	51.018	34.644	96.606	-162.619	107.448	-3.980
6000	16.000	51.287	34.920	98.206	-162.501	112.015	-4.080

31 December 1963 HLS

TITANIUM NITRIDE (TiN) (CONDENSED PHASE) gfw = 61.908

$\Delta H^{o}_{f\,298.15}$ = -80.750 kcal gfw^{-1} $S^{o}_{298.15}$ = 7.24 cal degK^{-1}gfw^{-1}

T_m = 3223°K ΔH_m = 15.0 kcal gfw^{-1}

$H^{o}_{298.15} - H^{o}_{0}$ = 1.310 kcal gfw^{-1}

C^{o}_{p} = 11.91 + 0.94 x 10^{-3}T -2.96 x 10^{5}T^{-2}cal degK^{-1}gfw^{-1} 298.15°K $\leq$ T $\leq$ 3223°K

C^{o}_{p} = 16.0 cal degK^{-1} gfw^{-1} 3223°K $\leq$ T $\leq$ 6000°K

Structure

TiN has a cubic structure (NaCl type) with a wide homogeneity range.

Heat of Formation

Combustion data of Humphrey[1] modified to be consistent with present compilation.

Heat Capacity and Entropy

Low-temperature data from Shomate.[2] High-temperature data of Naylor[3] valid to 1738°K extrapolated to melting point. Data above melting point estimated.

Melting and Vaporization

Heat of fusion estimated.

References

1. Humphrey, G. L., J. Am. Chem. Soc. 73, 2261 (1951).
2. Shomate, C. H., J. Am. Chem. Soc. 68, 310 (1946).
3. Naylor, B. F., J. Am. Chem. Soc. 68, 370 (1946).

TABLE 170

ZIRCONIUM NITRIDE. CONDENSED PHASE **NZr**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p:
Solid Zr from 0° to 2125°K, Liquid Zr from 2125° to 4644°K,
Gaseous Zr from 4644° to 6000°K; Gaseous N_2;
Solid ZrN from 0° to 3253°K,
Liquid ZrN from 3253° to 6000°K.

T, °K	C_p° (cal/°K gfw.)	S_T° (cal/°K gfw.)	$(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw.)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw.)	ΔH_f° (Kcal/gfw.)	ΔF_f° (Kcal/gfw.)	Log K_p
0	0.000	0.000	INFINITE	-1.575	-86.526	-86.526	INFINITE
298.15	9.666	9.290	9.290	0.000	-87.300	-80.477	58.988
300	9.693	9.350	9.290	0.018	-87.299	-83.434	58.594
400	10.697	12.293	9.685	1.043	-87.254	-78.151	42.698
500	11.252	14.744	10.459	2.143	-87.178	-75.884	33.167
600	11.630	16.831	11.351	3.288	-87.091	-73.633	26.820
700	11.925	18.647	12.266	4.466	-86.999	-71.397	22.290
800	12.175	20.256	13.166	5.672	-86.907	-69.175	18.897
900	12.400	21.703	14.036	6.900	-86.818	-66.964	16.260
1000	12.608	23.020	14.869	8.151	-86.730	-64.762	14.153
1100	12.806	24.231	15.666	9.422	-86.645	-62.570	12.431
1135	12.873	24.634	15.937	9.871	-86.615	-61.805	11.900
1135	12.873	24.634	15.937	9.871	-87.530	-61.805	11.900
1200	12.997	25.354	16.427	10.712	-87.464	-60.333	10.988
1300	13.182	26.402	17.155	12.021	-87.351	-58.077	9.763
1400	13.364	27.385	17.851	13.348	-87.224	-55.830	8.715
1500	13.544	28.313	18.518	14.694	-87.083	-53.593	7.808
1600	13.721	29.193	19.158	16.057	-86.928	-51.365	7.016
1700	13.896	30.030	19.773	17.438	-86.758	-49.147	6.318
1800	14.071	30.827	20.365	18.836	-86.574	-46.939	5.699
1900	14.244	31.595	20.936	20.252	-86.375	-44.743	5.146
2000	14.417	32.330	21.487	21.685	-86.161	-42.557	4.650
2100	14.589	33.037	22.021	23.135	-85.931	-40.384	4.203
2125	14.632	33.210	22.151	23.501	-85.870	-40.337	4.148
2125	14.632	33.210	22.151	23.501	-90.770	-40.337	4.148
2200	14.760	33.720	22.537	24.603	-90.593	-41.345	4.107
2300	14.941	34.380	23.038	26.087	-90.343	-35.664	3.389
2400	15.102	35.019	23.524	27.589	-90.077	-33.293	3.032
2500	15.272	35.649	23.996	29.108	-89.795	-30.931	2.704
2600	15.443	36.241	24.455	30.644	-89.497	-28.580	2.402
2700	15.612	36.827	24.903	32.196	-89.184	-26.248	2.124
2800	15.782	37.398	25.339	33.766	-88.854	-23.922	1.867
2900	15.952	37.955	25.764	35.353	-88.509	-21.605	1.628
3000	16.121	38.499	26.180	36.956	-88.148	-19.308	1.407
3100	16.290	39.030	26.586	38.577	[illegible]	-17.018	1.200
3200	16.455	39.550	26.983	40.214	[illegible]	-14.743	1.007
3253	16.549	39.821	27.190	41.089	-87.161	-13.543	0.910
3253	16.000	45.965	27.190	61.089	-67.161	-13.543	0.910
3300	16.000	46.197	27.459	61.841	-66.993	-12.768	0.846
3400	16.000	46.676	28.017	63.441	-66.638	-11.130	0.715
3500	16.000	47.140	28.557	65.041	-66.284	-9.502	0.593
3600	16.000	47.591	29.079	66.641	-65.930	-7.884	0.479
3700	16.000	48.029	29.586	68.241	-65.577	-6.277	0.371
3800	16.000	48.456	30.077	69.841	-65.224	-4.682	0.269
3900	16.000	48.871	30.553	71.441	-64.872	-3.087	0.173
4000	16.000	49.277	31.016	73.041	-64.5[illegible]	-1.508	0.082
4100	16.000	49.672	31.466	74.641	-64.169	0.063	-0.003
4200	16.000	50.057	31.905	76.241	-63.818	1.620	-0.084
4300	16.000	50.434	32.331	77.841	-63.468	3.178	-0.162
4400	16.000	50.801	32.747	79.441	-63.118	4.722	-0.235
4500	16.000	51.161	33.152	81.041	-62.769	6.262	-0.304
4600	16.000	51.513	33.547	82.641	-62.420	7.793	-0.370
4644.05	16.000	51.665	33.718	83.346	-62.265	8.467	-0.398
4644.05	16.000	51.665	33.718	83.346	-197.719	8.467	-0.398
4700	16.000	51.857	33.933	84.241	-197.579	10.949	-0.509
4800	16.000	52.194	34.310	85.841	-197.332	15.382	-0.700
4900	16.000	52.524	34.678	87.441	-197.091	19.816	-0.884
5000	16.000	52.847	35.039	89.041	-196.854	24.235	-1.059
5100	16.000	53.164	35.391	90.641	-196.623	28.651	-1.228
5200	16.000	53.474	35.736	92.241	-196.397	33.070	-1.390
5300	16.000	53.779	36.073	93.841	-196.176	37.483	-1.546
5400	16.000	54.078	36.404	95.441	-195.958	41.887	-1.695
5500	16.000	54.372	36.728	97.041	-195.743	46.287	-1.839
5600	16.000	54.660	37.046	98.641	-195.533	50.690	-1.978
5700	16.000	54.943	37.357	100.241	-195.326	55.086	-2.112
5800	16.000	55.222	37.663	101.841	-195.120	59.475	-2.241
5900	16.000	55.495	37.963	103.441	-194.918	63.864	-2.366
6000	16.000	55.764	38.257	105.041	-194.718	68.253	-2.486

31 December 1963 HLS

ZIRCONIUM NITRIDE (ZrN) (CONDENSED PHASE) gfw - 105.228

$\Delta H^{o}_{f298.15} = -87.3$ kcal gfw^{-1} $S^{o}_{298.15} = 9.29$ cal degK^{-1}gfw^{-1}

$T_m = 3253^{o}K$ $\Delta H_m = 20.0$ kcal gfw^{-1}

$H^{o}_{298.15} - H^{o}_{0} = 1.575$ kcal gfw^{-1}

$C^{o}_{p} = 11.10 + 1.68 \times 10^{-3}T - 1.72 \times 10^{5}T^{-2}$ cal degK^{-1}gfw^{-1} $298.15^{o}K \leq T \leq 3253^{o}K$

$C^{o}_{p} = 16.0$ cal degK^{-1} gfw^{-1} $3253^{o}K \leq T \leq 6000^{o}K$

Structure

ZrN has a cubic structure isotypic with NaCl. It has a fairly wide homogeneity range.

Heat of Formation

Based on the work of Mah and Gellert, [1] but in agreement with Neumann et al[2] and Smagina et al. [3]

Heat Capacity and Entropy

The low-temperature data of Todd[4] used. High-temperature data of Coughlin and King[5] extrapolated to melting point.

Melting and Vaporization

Melting temperature by Agte and Moers. [6]

References

1. Mah, A. D. and N. L. Gellert, J. Am. Chem. Soc. 78, 3261 (1956).
2. Neumann, B. et al, Z. Anorg. Chem. 218, 379 (1934).
3. Smagina, E. I. et al, Dokl. Akad. Nauk SSSR 115, 354 (1957).
4. Todd, S. S., J. Am. Chem. Soc. 72, 2914 (1950).
5. Coughlin, J. P. and E. G. King, J. Am. Chem. Soc. 72, 2262 (1950).
6. Agte, C. and K. Moers, Z. Anorg. Chem. 198, 239 (1931).

TABLE 171

NITROGEN

REFERENCE STATE

N_2

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p:
Gaseous Diatomic N_2 from 0° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.072			
298.15	6.961	45.771	45.771	0.000			
300	6.961	45.814	45.771	0.013			
400	6.991	47.820	46.045	0.710			
500	7.070	49.388	46.562	1.413			
600	7.197	50.687	47.144	2.126			
700	7.351	51.808	47.732	2.853			
800	7.513	52.800	48.305	3.596			
900	7.670	53.695	48.855	4.356			
1000	7.815	54.510	49.380	5.130			
1100	7.945	55.261	49.881	5.918			
1200	8.061	55.958	50.359	6.719			
1300	8.162	56.607	50.815	7.530			
1400	8.250	57.215	51.251	8.351			
1500	8.328	57.787	51.667	9.180			
1600	8.396	58.327	52.067	10.016			
1700	8.456	58.838	52.450	10.858			
1800	8.509	59.322	52.819	11.707			
1900	8.555	59.784	53.173	12.560			
2000	8.597	60.224	53.515	13.418			
2100	8.635	60.644	53.844	14.279			
2200	8.668	61.047	51.163	15.144			
2300	8.698	61.433	54.471	16.013			
2400	8.726	61.803	54.768	16.884			
2500	8.751	62.160	55.057	17.758			
2600	8.774	62.504	55.337	18.634			
2700	8.795	62.835	55.608	19.513			
2800	8.814	63.156	55.872	20.393			
2900	8.832	63.465	56.129	21.276			
3000	8.849	63.765	56.378	22.160			
3100	8.865	64.055	56.621	23.045			
3200	8.879	64.337	56.858	23.933			
3300	8.893	64.610	57.089	24.821			
3400	8.906	64.876	57.314	25.711			
3500	8.918	65.134	57.534	26.602			
3600	8.930	65.386	57.748	27.495			
3700	8.941	65.631	57.958	28.388			
3800	8.951	65.869	58.163	29.283			
3900	8.961	66.102	58.364	30.178			
4000	8.971	66.329	58.560	31.075			
4100	8.980	66.551	58.752	31.973			
4200	8.989	66.767	58.941	32.871			
4300	8.998	66.979	59.125	33.770			
4400	9.006	67.186	59.306	34.671			
4500	9.014	67.388	59.483	35.572			
4600	9.022	67.587	59.657	36.474			
4700	9.030	67.781	59.828	37.376			
4800	9.038	67.971	59.996	38.280			
4900	9.045	68.157	60.161	39.184			
5000	9.053	68.340	60.322	40.089			
5100	9.060	68.520	60.481	40.994			
5200	9.068	68.696	60.638	41.901			
5300	9.075	68.868	60.792	42.808			
5400	9.083	69.038	60.943	43.716			
5500	9.090	69.205	61.091	44.624			
5600	9.098	69.369	61.238	45.534			
5700	9.105	69.530	61.382	46.444			
5800	9.113	69.689	61.524	47.355			
5900	9.122	69.844	61.664	48.267			
6000	9.130	69.998	61.801	49.179			

May 1962 RCF

NITROGEN (N_2) (REFERENCE STATE) gfw = 28.016

ΔH°_{f0} = 0.0 kcal gfw^{-1}

$\Delta H^\circ_{f298.15}$ = 0.0 kcal gfw^{-1}

Ground State Configuration - $^1\Sigma_g^+$

$S^\circ_{298.15}$ = 45.771 cal degK^{-1} gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 2.072 kcal gfw^{-1}

State	g	E (cm^{-1})	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})	$\omega_e y_e$ (cm^{-1})	B_e (cm^{-1})	α_e (cm^{-1})	$\gamma_e \times 10^5$ (cm^{-1})	$D_e \times 10^6$ (cm^{-1})
X $^1\Sigma_g^+$	1	0.0	2357.93	14.186	-0.0124	1.9981	0.01709	-4.6	6
A $^3\Sigma_u^+$	3	49757.2	1460.19	13.888	-0.025	1.440	0.013	-	5.6
B $^3\Pi_g$	6	59314.2	1733.89	14.47	-	1.6376	0.0184	-	5.8

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Calculated on diatomic gas-computer program using above spectroscopic constants.[1]

Reference

1. Barriault, R. J., et al, ASD TR 61-620 (May 1962), Pt. 1.

NITROGEN (N_2) (REFERENCE STATE) GFW = 28.016

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal gfw)	ΔH_f (Kcal gfw)	ΔF_f (Kcal gfw)	Log K_p
298.15	±0.000	±0.002	±0.002	±0.000			
1000	±0.000	±0.003	±0.002	±0.000			
2000	±0.000	±0.003	±0.003	±0.001			
3000	±0.000	±0.004	±0.003	±0.001			
4000	±0.000	±0.004	±0.003	±0.001			
5000	±0.000	±0.004	±0.003	±0.001			
6000	±0.000	±0.004	±0.003	±0.001			

TABLE 172

SILICON NITRIDE — **CONDENSED PHASE** — **N_4Si_3**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p:
Solid Si from 0° to 1690°K, Liquid Si from 1690° to 3566°K,
Gaseous Si from 3566° to 6000°K; Gaseous N_2;
Solid Si_3N_4 from 0° to 4000°K.

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-5.598	-175.147	-175.147	INFINITE
298.15	30.900	25.600	25.600	0.000	-176.000	-152.288	111.624
300	30.941	25.791	25.601	0.057	-175.996	-152.141	110.829
400	32.544	34.935	26.836	3.239	-175.732	-144.228	78.799
500	33.542	42.311	29.217	6.547	-175.477	-136.383	59.610
600	34.304	48.496	31.929	9.940	-175.232	-128.587	46.836
700	34.953	53.834	34.685	13.404	-174.995	-120.832	37.724
800	35.542	58.540	37.379	16.929	-174.771	-113.111	30.899
900	36.097	62.758	39.968	20.511	-174.560	-105.416	25.597
1000	36.629	66.589	42.442	24.147	-174.359	-97.743	21.361
1100	37.148	70.105	44.799	27.836	-174.163	-90.091	17.899
1200	37.657	73.359	47.045	31.577	-173.971	-82.458	15.017
1300	38.160	76.393	49.187	35.368	-173.776	-74.838	12.581
1400	38.657	79.239	51.233	39.209	-173.578	-67.234	10.495
1500	39.151	81.923	53.191	43.099	-173.377	-59.647	8.690
1600	39.642	84.466	55.066	47.039	-173.164	-52.069	7.112
1690	40.083	86.647	56.691	50.626	-172.965	-45.268	5.854
1690	40.083	86.647	56.691	50.626	-208.815	-45.268	5.854
1700	40.131	86.884	56.868	51.027	-208.787	-44.299	5.695
1800	40.619	89.191	58.600	55.065	-208.558	-34.626	4.204
1900	41.105	91.400	60.268	59.151	-208.311	-24.971	2.872
2000	41.590	93.521	61.878	63.286	-208.043	-15.328	1.675
2100	42.074	95.562	63.434	67.469	-207.727	-5.703	0.593
2200	42.557	97.531	64.939	71.701	-207.373	-9.288	0.923
2300	43.040	99.433	66.398	75.980	-206.977	13.504	-1.283
2400	43.522	101.275	67.813	80.308	-206.539	23.078	-2.101
2500	44.004	103.061	69.187	84.685	-206.055	32.637	-2.853
2600	44.485	104.797	70.524	89.109	-205.531	42.176	-3.545
2700	44.966	106.484	71.824	93.582	-204.961	51.688	-4.184
2800	45.447	108.128	73.092	98.103	-204.348	61.182	-4.775
2900	45.928	109.732	74.328	102.671	-203.691	70.657	-5.325
3000	46.408	111.297	75.534	107.288	-202.990	80.107	-5.836
3100	46.889	112.826	76.712	111.953	-202.249	89.530	-6.312
3200	47.369	114.323	77.864	116.666	-201.451	98.931	-6.756
3300	47.849	115.788	78.992	121.427	[illegible]	108.305	-7.172
3400	48.329	117.223	80.095	126.236	[illegible]	117.658	-7.563
3500	48.809	118.631	81.176	131.092	[illegible]	126.981	-7.929
3565.77	49.124	119.543	81.875	134.313	-198.164	133.092	-8.157
3565.77	49.124	119.543	81.875	134.313	-472.649	133.092	-8.157
3600	49.288	120.013	82.236	135.997	-472.141	138.903	-8.432
3700	49.768	121.370	83.275	140.950	-470.627	155.860	-9.206
3800	50.247	122.703	84.295	145.951	-469.072	172.772	-9.936
3900	50.727	124.015	85.297	151.000	-467.469	189.637	-10.626
4000	51.206	125.305	86.281	156.036	-465.820	206.472	-11.281

31 December 1963 — HLS

SILICON NITRIDE (Si_3N_4) (CONDENSED PHASE) gfw = 140. 302

ΔHf^o_{298} = -176. 0 kcal gfw^{-1} $S^o_{298.15}$ = 25. 6 cal $degK^{-1}gfw^{-1}$

$T_{sublimation}$ = 2170°K

$H^o_{298.15} - H^o_0$ = 5. 598 kcal gfw^{-1}

$C^o_p = 32.074 + 0.0047867T - 0.23122 \times 10^6 T^{-2}$ cal $degK^{-1}gfw^{-1}$ $298.15°K \leq T \leq 4000°K$

Structure

α - Si_3N_4 is probably hexagonal as is β - Si_3N_4 .

Heat of Formation

Based on dissociation-pressure measurements of Pehlke and Elliott.[1]

Heat Capacity and Entropy

Low-and high-temperature data estimated by Pehlke and Elliott.[1] An equation derived based on their data and extrapolated. Experimental enthalpies of Neel et al[2] somewhat larger than the estimated values used here.

Melting and Vaporization

Si_3N_4 considered to sublime rather than melt.

References

1. Pehlke, R. D. and J. F. Elliott, Trans. AIME 215, 781 (1959).
2. Neel, D. S. et al, WAD TR 60-924 (1962).

SILICON NITRIDE (Si_3N_4) (CONDENSED PHASE). GFW = 140.302

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal °K gfw)	S^o_T (cal °K gfw)	$-(F^o_T - H^o_{298})/T$ (cal °K gfw)	$H^o_T - H^o_{298}$ (kcal gfw)	ΔH_f (kcal gfw)	ΔF_f (kcal gfw)	Log K_p
298.15	±5.000	±4.000	± 4.000	± 0.000	±6.000		
500	±5.000	±6.585	± 4.567	± 1.009			
1000	±5.000	±10.051	± 6.542	± 3.509			
1500	±5.000	±12.078	± 8.072	± 6.009			
1690	±5.000	±12.674	± 8.557	± 6.959			
2000	±5.000	±13.517	± 9.262	± 8.509			
2500	±5.000	±14.632	±10.229	±11.009			
3000	±5.000	±15.544	±11.041	±13.509			
3500	±5.000	±16.315	±11.741	±16.009			
3565.77	±5.000	±16.408	±11.826	±16.338			
4000	±5.000	±16.982	±12.355	±18.509			

TABLE 173

NIOBIUM **REFERENCE STATE** **Nb**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p. Solid Nb from 0° to 2741°K, Liquid Nb from 2741° to 5032°K, Gaseous Nb from 5032° to 6000°K.

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.264			
298.15	5.946	9.000	9.000	0.000			
300	5.948	9.037	9.000	0.011			
400	6.044	10.761	9.235	0.611			
500	6.140	12.120	9.680	1.220			
600	6.236	13.248	10.184	1.839			
700	6.332	14.216	10.692	2.467			
800	6.428	15.068	11.187	3.105			
900	6.524	15.831	11.661	3.753			
1000	6.620	16.523	12.113	4.410			
1100	6.716	17.159	12.544	5.077			
1200	6.812	17.747	12.953	5.753			
1300	6.908	18.296	13.343	6.439			
1400	7.004	18.812	13.716	7.135			
1500	7.100	19.298	14.072	7.840			
1600	7.196	19.759	14.413	8.555			
1700	7.292	20.199	14.740	9.279			
1800	7.388	20.618	15.055	10.013			
1900	7.484	21.020	15.359	10.757			
2000	7.580	21.406	15.652	11.510			
2100	7.676	21.779	15.935	12.273			
2200	7.772	22.138	16.208	13.045			
2300	7.868	22.486	16.474	13.827			
2400	7.964	22.822	16.731	14.619			
2500	8.060	23.149	16.982	15.420			
2600	8.156	23.467	17.225	16.231			
2700	8.252	23.777	17.462	17.051			
2741	8.291	23.902	17.557	17.390			
2741	8.000	26.237	17.557	23.790			
2800	8.000	26.407	17.742	24.262			
2900	8.000	26.688	18.046	25.062			
3000	8.000	26.959	18.338	25.862			
3100	8.000	27.221	18.621	26.662			
3200	8.000	27.475	18.893	27.462			
3300	8.000	27.721	19.157	28.262			
3400	8.000	27.960	19.413	29.062			
3500	8.000	28.192	19.660	29.862			
3600	8.000	28.418	19.900	30.662			
3700	8.000	28.637	20.133	31.462			
3800	8.000	28.850	20.360	32.262			
3900	8.000	29.058	20.580	33.062			
4000	8.000	29.260	20.795	33.862			
4100	8.000	29.458	21.004	34.662			
4200	8.000	29.651	21.207	35.462			
4300	8.000	29.839	21.406	36.262			
4400	8.000	30.023	21.600	37.062			
4500	8.000	30.203	21.789	37.862			
4600	8.000	30.379	21.974	38.662			
4700	8.000	30.551	22.154	39.462			
4800	8.000	30.719	22.331	40.262			
4900	8.000	30.884	22.504	41.062			
5000	8.000	31.046	22.673	41.862			
5031.58	8.000	31.062	22.713	42.115			
5031.58	8.600	63.393	22.713	204.688			
5100	8.640	63.510	23.260	205.277			
5200	8.695	63.678	24.036	206.144			
5300	8.749	63.844	24.785	207.016			
5400	8.800	64.008	25.510	207.893			
5500	8.848	64.170	26.211	208.776			
5600	8.895	64.330	26.890	209.663			
5700	8.939	64.488	27.548	210.555			
5800	8.981	64.644	28.187	211.451			
5900	9.021	64.798	28.806	212.351			
6000	9.059	64.950	29.407	213.255			

15 March 1963 HLS

$0^\circ K$ to $2741^\circ K$	Crystal
$2741^\circ K$ to $5032^\circ K$	Liquid
$5032^\circ K$ to $6000^\circ K$	Ideal Monatomic Gas

$\Delta H^\circ_{f0} = 0$

$\Delta H^\circ_{f298.15} = 0$

$\Delta H^\circ_{s298.15} = 171.836$ Kcal gfw^{-1}

$S^\circ_{298.15} = 9.0$ cal degK^{-1} gfw^{-1}

$T_m = 2741^\circ K$

$\Delta H_m = 6.400 \pm 1.000$ Kcal gfw^{-1} (Estd.)

$T_b = 5031.58^\circ K$

$\Delta H_v = 162.573$ Kcal gfw^{-1}

$H^\circ_{298.15} - H^\circ_0 = 1.264$ Kcal gfw^{-1}

$C^\circ_p = 5.66 + 0.96 \times 10^{-3} T$ cal deg^{-1} gfw^{-1} for $298.15^\circ K \leq T \leq 2741^\circ K$

$C^\circ_p = 8.00 \pm 2.0$ cal deg^{-1} gfw^{-1} for liquid ($2741^\circ K \leq T \leq 5032^\circ K$) (Estd.)

Structure

Solid has a B.C.C. type structure.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Entropy at $298.15^\circ K$ from Kelley and King [1] High-temperature data of Kelley [2] was extrapolated.

Melting

Temperature of fusion from Schofield [3] Heat of fusion estimated by Kelley [2] and by Stull and Sinke [4]

Heat of Sublimation

Data of Speiser *et al* [5] was used.

References

1. Kelley, K. K. and E. G. King, U. S. Bur. Mines, Bull. 592 (1961)
2. Kelley, K. K., U. S. Bur. Mines, Bull. 584 (1960).
3. Schofield, T. H., J. Inst. Metals 85, 372 (1957).
4. Stull, D. R. and G. C. Sinke, Thermodynamic Properties of the Elements (1956).
5. Speiser, R., P. Blackburn and H. L. Johnston, J. Electrochem Soc. 106, 52-3 (1959).

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw C°_p	S°_T	$-(F^\circ_T - H^\circ_{298})/T$	Kcal/gfw $H^\circ_T - H^\circ_{298}$	ΔH°_f	ΔF°_f	Log K_p
298.15	±0.100	±0.400	±0.400	±0.000			
1000	±0.300	±0.660	±0.489	±0.170			
2000	±0.500	±0.925	±0.640	±0.570			
2741	±1.000	±1.129	±0.742	±1.061			
2741	±2.000	±1.494	±0.742	±2.061			
3000	±2.000	±1.674	±0.814	±2.579			
4000	±2.000	±2.250	±1.105	±4.579			
5000	±2.000	±2.696	±1.380	±6.579			
5031.58	±2.000	±2.708	±1.388	±6.642			

NIOBIUM — IDEAL MONATOMIC GAS — Nb

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Nb from 0° to 2741°K, Liquid Nb from 2741° to 5032°K, Gaseous Nb from 5032° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.997	171.103	171.103	INFINITE
298.15	7.208	44.492	44.492	0.000	171.836	161.254	-118.197
300	7.208	44.537	44.492	0.013	171.838	161.188	-117.420
400	7.086	46.597	44.774	0.729	171.954	157.620	-86.116
500	6.893	48.157	45.301	1.428	172.044	154.026	-67.321
600	6.704	49.397	45.884	2.108	172.105	150.416	-54.786
700	6.541	50.418	46.461	2.770	172.139	146.798	-45.830
800	6.402	51.282	47.011	3.417	172.148	143.177	-39.112
900	6.285	52.029	47.528	4.051	172.134	139.556	-33.887
1000	6.186	52.686	48.012	4.674	172.100	135.937	-29.708
1100	6.103	53.272	48.464	5.289	172.048	132.324	-26.289
1200	6.035	53.800	48.887	5.895	171.978	128.716	-23.441
1300	5.981	54.280	49.283	6.496	171.893	125.114	-21.032
1400	5.941	54.722	49.656	7.092	171.793	121.520	-18.969
1500	5.915	55.131	50.008	7.685	171.681	117.932	-17.182
1600	5.903	55.512	50.340	8.276	171.557	114.353	-15.619
1700	5.904	55.870	50.655	8.866	171.423	110.781	-14.241
1800	5.918	56.208	50.954	9.457	17[illegible].280	107.218	-13.017
1900	5.945	56.528	51.239	10.050	171.129	103.664	-11.923
2000	5.984	56.834	51.511	10.646	170.972	100.117	-10.940
2100	6.034	57.127	51.772	11.247	170.810	96.579	-10.051
2200	6.094	57.409	52.022	11.853	170.644	93.046	-9.243
2300	6.164	57.682	52.262	12.466	170.475	89.524	-8.506
2400	6.242	57.946	52.493	13.086	170.303	86.007	-7.832
2500	6.328	58.202	52.716	13.715	170.131	82.500	-7.212
2600	6.419	58.452	52.932	14.352	169.957	78.997	-6.640
2700	6.516	58.696	53.141	14.999	169.784	75.502	-6.111
2741	6.556	58.795	53.225	15.267	169.713	74.070	-5.906
2741	6.556	58.795	53.225	15.267	163.313	74.070	-5.906
2800	6.616	58.935	53.344	15.655	163.229	72.150	-5.631
2900	6.719	59.169	53.541	16.322	163.096	68.901	-5.192
3000	6.825	59.399	53.732	16.999	162.973	65.653	-4.783
3100	6.931	59.624	53.919	17.687	162.861	62.413	-4.400
3200	7.038	59.846	54.100	18.385	162.759	59.172	-4.041
3300	7.144	60.064	54.278	19.095	162.669	55.937	-3.704
3400	7.250	60.279	54.451	19.814	162.588	52.706	-3.388
3500	7.354	60.491	54.621	20.545	162.519	49.473	-3.089
3600	7.456	60.699	54.787	21.285	162.[illegible]9	46.244	-2.807
3700	7.555	60.905	54.949	22.036	162.410	43.016	-2.541
3800	7.652	61.108	55.109	22.796	162.370	39.791	-2.288
3900	7.747	61.308	55.265	23.566	162.340	36.564	-2.049
4000	7.838	61.505	55.419	24.345	162.319	33.341	-1.822
4100	7.926	61.700	55.569	25.133	162.307	30.118	-1.605
4200	8.011	61.892	55.718	25.930	162.304	26.891	-1.399
4300	8.093	62.081	55.863	26.736	162.310	23.669	-1.203
4400	8.172	62.268	56.007	27.549	162.323	20.445	-1.015
4500	8.247	62.453	56.148	28.370	162.344	17.220	-0.836
4600	8.320	62.635	56.287	29.198	162.372	13.995	-0.665
4700	8.390	62.814	56.424	30.034	162.408	10.766	-0.501
4800	8.456	62.992	56.559	30.876	162.450	7.541	-0.343
4900	8.520	63.167	56.692	31.725	162.499	4.314	-0.192
5000	8.581	63.339	56.823	32.580	162.554	1.084	-0.047
5031.58	8.600	63.393	56.864	32.851	162.572	0.000	-0.000
5031.58	8.600	63.393	56.864	32.851			
5100	8.640	63.510	56.953	33.441			
5200	8.695	63.678	57.081	34.308			
5300	8.749	63.844	57.207	35.180			
5400	8.800	64.008	57.331	36.057			
5500	8.848	64.170	57.454	36.940			
5600	8.895	64.330	57.575	37.827			
5700	8.939	64.488	57.695	38.719			
5800	8.981	64.644	57.814	39.615			
5900	9.021	64.798	57.931	40.515			
6000	9.059	64.950	58.046	41.419			

15 March 1963 — HLS

ΔH^{o}_{f0} = 171.103 Kcal gfw^{-1}

Ground State Configuration $^{6}D_{\frac{1}{2}}$

$H^{o}_{298.15}-H^{o}_{0}$ = 1.997 Kcal gfw^{-1}

$\Delta H^{o}_{f298.15}$ = 171.836 Kcal gfw^{-1}

$S^{o}_{298.15}$ = 44.492 cal degK^{-1} gfw^{-1}

Electronic Levels and Multiplicities

All energy levels listed by Moore[1]

Heat of Formation

Vapor-pressure data of Speiser et al[2] were used.

Heat Capacity and Entropy

Calculated using the monatomic gas program.

References

1. Moore, C. E., Natl. Bur. Standards (U.S.), Circ. 467, Vol. 2 (1952).
2. Speiser, R., P. Blackburn and H. L. Johnston, J. Electrochem. Soc. 106, 52 (1959).

NIOBIUM, MONATOMIC (Nb) (IDEAL GAS) GFW = 92.91

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal °K gfw			Kcal gfw			
	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f^o	ΔF_f^o	Log K_p
298.15	±0.001	±0.002	±0.003	±0.000	±4.000		
1000	±0.000	±0.003	±0.003	±0.000			
2000	±0.000	±0.003	±0.003	±0.001			
3000	±0.001	±0.003	±0.003	±0.001			
4000	±0.002	±0.003	±0.003	±0.002			
5000	±0.002	±0.004	±0.003	±0.004			
5031.58	±0.002	±0.004	±0.003	±0.004			
6000	±0.003	±0.004	±0.003	±0.006			

TABLE 175

NIOBIUM MONOXIDE — CONDENSED PHASE — **NbO**

Reference State for Calculating ΔH_f°, ΔF_f°, Log K_p: Solid Nb from 0° to 2741°K, Liquid Nb from 2741° to 5032°K, Gaseous Nb from 5032° to 6000°K, Gaseous O_2. Solid NbO from 0° to 2218°K, Liquid NbO from 2218° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.800	-97.198	-97.198	INFINITE
298.15	9.860	12.000	12.000	0.000	-97.700	-91.289	66.913
300	9.875	12.061	12.000	0.018	-97.699	-91.249	66.472
400	10.491	14.994	12.396	1.039	-97.633	-89.108	48.684
500	10.902	17.381	13.162	2.110	-97.537	-86.987	38.020
600	11.232	19.399	14.037	3.217	-97.427	-84.887	30.918
700	11.525	21.153	14.931	4.355	-97.305	-82.807	25.852
800	11.798	22.710	15.808	5.521	-97.176	-80.744	22.057
900	12.058	24.114	16.654	6.714	-97.038	-78.699	19.110
1000	12.312	25.398	17.465	7.933	-96.890	-76.668	16.755
1100	12.560	26.583	18.241	9.176	-96.734	-74.653	14.832
1200	12.806	27.687	18.983	10.445	-96.565	-72.654	13.232
1300	13.049	28.721	19.692	11.737	-96.387	-70.668	11.880
1400	13.290	29.697	20.372	13.054	-96.198	-68.696	10.723
1500	13.530	30.622	21.025	14.395	-95.997	-66.739	9.723
1600	13.769	31.503	21.653	15.760	-9[illegible].786	-64.797	8.850
1700	14.008	32.345	22.257	17.149	-95.567	-62.867	8.082
1800	14.246	33.152	22.840	18.562	-95.328	-60.950	7.400
1900	14.483	33.929	23.403	19.998	-95.083	-59.045	6.791
2000	14.720	34.678	23.949	21.459	-94.825	-57.156	6.245
2100	14.957	35.402	24.477	22.943	-94.557	-55.279	5.753
2200	15.194	36.103	24.989	24.450	-94.277	-53.415	5.306
2218	15.236	36.227	25.080	24.724	-94.226	-53.083	5.230
2218	15.000	42.088	25.080	37.724	-81.226	-53.083	5.230
2300	15.000	42.633	25.696	38.954	-81.013	-52.044	4.945
2400	15.000	43.271	26.415	40.454	-80.766	-50.791	4.625
2500	15.000	43.884	27.102	41.954	-80.531	-49.546	4.331
2600	15.000	44.472	27.759	43.454	-80.308	-48.312	4.061
2700	15.000	45.038	28.388	44.954	-80.097	-47.084	3.811
2741	15.000	45.264	28.639	45.569	-80.014	-46.586	3.714
2741	15.000	45.264	28.639	45.569	-86.414	-46.586	3.714
2800	15.000	45.583	28.993	46.454	-86.279	-45.729	3.569
2900	15.000	46.110	29.574	47.954	-86.053	-44.283	3.337
3000	15.000	46.618	30.134	49.454	-85.829	-42.850	3.121
3100	15.000	47.110	30.673	50.954	[illegible]	-41.415	2.920
3200	15.000	47.586	31.195	52.454	-85.39[illegible]	-39.999	2.732
3300	15.000	48.048	31.698	53.954	[illegible]	-38.581	2.555
3400	15.000	48.496	32.186	55.454	-84.956	-37.172	2.389
3500	15.000	48.931	32.658	56.954	-84.743	-35.769	2.233
3600	15.000	49.353	33.116	58.454	-84.532	-34.374	2.087
3700	15.000	49.764	33.560	59.754	-84.323	-32.993	1.948
3800	15.000	50.164	33.992	61.454	-84.115	-31.597	1.817
3900	15.000	50.554	34.412	62.954	-83.910	-30.220	1.693
4000	15.000	50.934	34.820	64.454	-83.706	-28.842	1.576
4100	15.000	51.304	35.218	65.954	-83.5[illegible]4	-27.475	1.464
4200	15.000	51.665	35.605	67.454	-83.304	-26.111	1.359
4300	15.000	52.018	35.983	68.954	-83.105	-24.751	1.258
4400	15.000	52.363	36.351	70.454	-82.909	-23.393	1.162
4500	15.000	52.700	36.711	71.954	-82.715	-22.046	1.071
4600	15.000	53.030	37.062	73.454	-82.523	-20.696	0.983
4700	15.000	53.353	37.405	74.954	-82.333	[illegible]9.356	0.900
4800	15.000	53.668	37.740	76.454	-82.147	-18.013	0.820
4900	15.000	53.978	38.069	77.754	-81.964	-16.681	0.744
5000	15.000	54.281	38.390	79.454	-81.784	-15.350	0.671
5031.58	15.000	54.375	38.490	79.928	-81.728	-14.993	0.651
5031.58	15.000	54.375	38.490	79.928	-244.301	-14.993	0.651
5100	15.000	54.578	38.704	80.954	-244.224	-11.872	0.509
5200	15.000	54.869	39.012	82.454	-244.121	-7.314	0.307
5300	15.000	55.155	39.314	83.954	-244.029	-2.764	0.114
5400	15.000	55.435	39.610	85.454	-243.950	1.790	-0.072
5500	15.000	55.710	39.901	86.954	-243.886	6.335	-0.252
5600	15.000	55.981	40.185	88.454	-243.836	10.887	-0.425
5700	15.000	56.246	40.465	89.954	-243.804	15.434	-0.592
5800	[illegible]	56.507	40.739	91.454	-243.792	19.991	-0.753
5900	15.000	56.763	41.009	92.954	-243.803	24.536	-0.909
6000	[illegible]	57.016	41.273	94.454	-243.839	29.092	-1.060

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NIOBIUM MONOXIDE (NbO) (CONDENSED PHASE) gfw = 108.91

$\Delta H^\circ_{f298.15}$ = -97.7 kcal gfw^{-1} $S^\circ_{298.15}$ = 12.0 ± 1.5 cal deg K^{-1}gfw^{-1}

T_m = 2218°K ΔH_m = 13.0 ± 4.0 kcal gfw^{-1}

$H^\circ_{298.15}-H^\circ_0$ = 1.800 kcal gfw^{-1}

$C^\circ_p = 10.04 + 2.35 \times 10^{-3}T - 0.783 \times 10^5 T^{-2}$ cal deg K^{-1}gfw^{-1} 298.15°K ≤ T ≤ 2218°K

C°_p = 15.0 cal deg K^{-1}gfw^{-1} 2218°K ≤ T ≤ 6000°K

Structure

NbO has a cubic (NaCl type) lattice with ordered vacancies.

Heat of Formation

An average, rounded value based on two calorimetric and two equilbria determinations.[1-4]

Heat Capacity and Entropy

Low temperature data estimated. High temperature data from Gel'd and Kusenko[5] up to 1800°K. Data at higher temperatures are estimated.

Melting and Vaporization

Melting temperature is from Elliott.[6] Heat of fusion is estimated.

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NIOBIUM MONOXIDE (NbO) (CONDENSED PHASE) GFW = 108.91

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw			Kcal/gfw			
	C°_p	S°_T	$(F^\circ_T - H^\circ_{298})/T$	$H^\circ_T - H^\circ_{298}$	ΔH°_f	ΔF°_f	Log K_p
298.15	±0.500	±1.500	±1.500	±0.000	±2.000		
1000	±0.500	±2.105	±1.754	±0.351			
1500	±0.500	±2.308	±1.907	±0.601			
1500	±1.000	±2.308	±1.907	±0.601			
2000	±1.000	±2.595	±2.045	±1.101			
2218	±1.000	±2.699	±2.104	±1.319			
2218	±2.000	±4.502	±2.104	±5.319			
3000	±2.000	±5.106	±2.812	±6.883			
4000	±2.000	±5.682	±3.461	±8.883			
5000	±2.000	±6.128	±3.951	±10.883			
6000	±2.000	±6.493	±4.346	±12.883			

TABLE 176

NIOBIUM MONOXIDE

IDEAL MOLECULAR GAS

NbO

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p. Solid Nb from 0° to 2741°K, Liquid Nb from 2741° to 5032°K, Gaseous Nb from 5032° to 6000°K; Gaseous O_2; Gaseous NbO.

T, °K	cal/°K gfw			Kcal/gfw			Log K_p
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	
0	0.000	0.000	INFINITE	-2.099	46.219	46.219	INFINITE
298.15	7.358	57.091	57.091	0.000	46.017	38.984	-28.575
300	7.366	57.136	57.091	0.014	46.013	38.941	-28.367
400	7.735	59.307	57.384	0.769	45.813	36.614	-20.004
500	8.034	61.067	57.950	1.558	45.628	34.335	-15.007
600	8.254	62.552	58.597	2.373	45.446	32.094	-11.690
700	8.413	63.837	59.255	3.207	45.263	29.883	- .330
800	8.530	64.968	59.900	4.054	45.073	27.699	-7.567
900	8.618	65.978	60.520	4.912	44.876	25.539	-6.201
1000	8.686	66.890	61.113	5.777	44.670	23.400	-5.114
1100	8.739	67.720	61.676	6.649	44.456	21.285	-4.229
1200	8.782	68.483	62.212	7.525	44.232	19.188	-3.494
1300	8.817	69.187	62.722	8.405	43.997	17.110	-2.876
1400	8.847	69.842	63.207	9.288	43.752	15.052	-2.350
1500	8.872	70.453	63.670	10.174	43.498	13.010	-1.896
1600	8.893	71.026	64.112	11.062	43.[illegible]	10.986	-1.501
1700	8.913	71.566	64.535	11.953	42.958	8.977	-1.154
1800	8.931	72.076	64.940	12.845	42.677	6.987	-0.848
1900	8.947	72.559	65.328	13.739	42.375	5.014	-0.577
2000	8.963	73.018	65.701	14.634	42.067	3.057	-0.334
2100	8.979	73.456	66.060	15.531	41.748	1.114	-0.116
2200	8.994	73.874	66.406	16.430	41.419	-0.815	0.081
2300	9.011	74.275	66.740	17.330	41.079	-2.728	0.259
2400	9.029	74.658	67.062	18.232	40.728	-4.627	0.421
2500	9.048	75.027	67.373	19.136	40.367	-6.507	0.569
2600	9.069	75.383	67.674	20.042	39.996	-8.374	0.704
2700	9.092	75.726	67.966	20.950	39.615	-10.228	0.828
2741	9.102	75.863	68.083	21.323	39.456	-10.985	0.876
2741	9.102	75.863	68.083	21.323	33.056	-10.985	0.876
2800	9.118	76.057	68.249	21.860	32.843	-11.929	0.931
2900	9.146	76.377	68.524	22.773	32.482	-13.521	1.019
3000	9.177	76.688	68.791	23.690	32.123	-15.103	1.100
3100	9.211	76.989	69.051	24.609	31.764	-16.670	1.175
3200	9.248	77.283	69.304	25.532	31.406	-18.231	1.245
3300	9.288	77.568	69.550	26.459	31.[illegible]	-19.775	1.310
3400	9.332	77.846	69.790	[illegible].390	30.696	-21.308	1.370
3500	9.379	78.117	70.024	20.325	30.34[illegible]	-22.833	1.426
3600	9.429	78.382	70.253	29.265	29.995	-24.350	1.478
3700	9.482	78.642	70.476	30.211	29.651	-25.855	1.527
3800	9.539	78.895	70.695	31.162	29.309	-27.351	1.573
3900	9.598	79.144	70.908	32.119	28.972	-28.838	1.616
4000	9.661	79.388	71.118	33.0d2	28.639	-30.317	1.656
4100	9.726	79.628	71.322	34.051	28.310	-31.785	1.694
4200	9.794	79.863	71.523	35.027	27.986	-33.250	1.730
4300	9.865	80.094	71.720	36.010	27.668	-34.703	1.764
4400	9.938	80.322	71.913	37.000	27.35[illegible]	-36.149	1.795
4500	10.013	80.547	72.103	37.997	27.045	-37.593	1.826
4600	10.090	80.768	72.289	39.003	26.743	-39.023	1.854
4700	10.168	80.986	72.472	40.015	[illegible].444	-40.454	1.881
4800	10.249	81.201	72.652	41.036	26.152	-41.873	1.906
4900	10.330	81.414	72.829	42.065	25.864	-4[illegible].288	1.931
5000	10.413	81.623	73.003	3.102	25.581	-4[illegible].698	1.954
5031.58	10.440	81.689	73.057	43.431	25.491	-45.203	1.963
5031.58	10.440	81.689	73.057	43.431	-137.081	-45.203	1.963
5100	10.497	81.831	73.174	44.147	-137.314	-43.952	1.883
5200	10.582	82.036	73.343	45.201	-137.657	-42.118	1.770
5300	10.667	82.238	73.510	46.263	-138.003	-40.286	1.661
5400	10.753	82.439	73.673	47.334	-138.354	-38.434	1.555
5500	10.839	82.637	73.835	48.413	-138.710	-36.585	1.454
5600	10.925	82.834	73.994	49.501	-139.072	-34.727	1.355
5700	11.012	83.028	74.152	50.598	-139.443	-32.865	1.260
5800	11.098	83.221	74.307	51.703	-139.826	-30.987	1.168
5900	11.184	83.412	74.460	52.816	-140.224	-29.108	1.078
6000	11.269	83.601	74.611	53.939	-140.637	-27.219	0.991

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ΔH°_{f0} = + 46.219 kcal gfw^{-1}

$\Delta H^\circ_{f298.15}$ = + 46.017 kcal gfw^{-1}

Ground State Configuration $^2\Lambda$

$S^\circ_{298.15}$ = 57.091 cal deg^{-1}gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 2.099 kcal gfw^{-1}

State	g	E (cm^{-1})	ω_e (cm^{-1})	$\omega_e x_e$ (cm^{-1})	$\omega_e y_e$ (cm^{-1})	B_e (cm^{-1})	α_e (cm^{-1})	$\gamma_e \times 10^5$ (cm^{-1})	$D_e \times 10^6$ (cm^{-1})
$X^2\Lambda$	4	0.0	989.03	3.83		0.4323	0.0024	-	0.26
C	4	15,400	919.5	20.3	-	0.41	-	-	-
B	4	18,280	998.	16.0	-	0.41	-	-	-
$A^2\Lambda$	4	21,385.3	850.48	3.37	-	0.4003	0.0020	-	0.30

Heat of Formation

Based on work of Shchukarev et al.[1]

Heat Capacity and Entropy

Calculated using constants shown above.[2-5]

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NIOBIUM MONOXIDE (NbO) (IDEAL MOLECULAR GAS) GFW = 108.91

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal gfw)	ΔH°_f (Kcal gfw)	ΔF°_f (Kcal gfw)	Log K_p
298.15	±1.000	±1.000	±1.000	±0.000	±5.000		
1000	±1.000	±2.210	±1.508	±0.702			
2000	±1.000	±2.903	±2.052	±1.702			
3000	±1.000	±3.309	±2.408	±2.702			
4000	±1.000	±3.596	±2.671	±3.702			
5000	±1.000	+3.820	±2.879	±4.702			
6000	±1.000	±4.002	±3.052	±5.702			

TABLE 177

NIOBIUM DIOXIDE — **CONDENSED PHASE** — NbO_2

Reference State for Calculating ΔH_f°, ΔF_f°, and Log Kp: Solid Nb from 0° to 2741°K, α-NbO_2 from 0° to 1090°K, β-NbO_2 from 1090° to 1200°K, γ-NbO_2 from 1200° to 2270°K, Liquid NbO_2 from 2270° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.222	-189.083	-189.083	INFINITE
298.15	13.740	13.030	13.030	0.000	-190.200	-176.790	129.584
300	13.768	13.115	13.030	0.025	-190.199	-176.707	128.725
400	15.074	17.262	13.587	1.470	-190.064	-172.227	94.096
500	16.192	20.748	14.679	3.034	-189.840	-167.792	73.339
600	17.236	23.793	15.949	4.706	-189.543	-163.409	59.519
700	18.245	26.526	17.268	6.480	-189.174	-159.082	49.665
800	19.235	29.027	18.584	8.354	-188.736	-154.813	42.291
900	20.215	31.349	19.875	10.327	-188.225	-150.603	36.570
1000	21.188	33.530	21.132	12.397	-187.640	-146.452	32.006
1090	22.060	35.393	22.233	14.343	-187.049	-142.770	28.625
1090	22.200	36.053	22.233	15.063	-186.329	-142.770	28.625
1100	22.200	36.256	22.360	15.285	-186.258	-142.371	28.285
1200	22.200	38.187	23.600	17.505	-185.562	-138.413	25.207
1200	19.850	38.187	23.600	17.505	-185.562	-138.413	25.207
1300	19.850	39.776	24.784	19.490	-185.120	-134.503	22.611
1400	19.850	41.247	25.908	21.475	-184.695	-130.624	20.390
1500	19.850	42.617	26.977	23.460	-184.285	-126.777	18.471
1600	19.850	43.898	27.995	25.445	-183.892	-122.957	16.794
1700	19.850	45.101	28.966	27.430	-183.514	-119.160	15.318
1800	19.850	46.236	29.894	29.415	-183.152	-115.385	14.009
1900	19.850	47.309	30.783	31.400	-182.805	-111.629	12.840
2000	19.850	48.327	31.635	33.385	-182.473	-107.890	11.789
2100	19.850	49.296	32.453	35.370	-182.157	-104.169	10.841
2200	19.850	50.219	33.240	37.355	-181.855	-100.464	9.980
2270	19.850	50.841	33.773	38.745	-181.652	-97.877	9.423
2270	20.000	57.449	33.773	53.745	-166.652	-97.877	9.423
2300	20.000	57.712	34.083	54.345	-166.563	-96.967	9.214
2400	20.000	58.563	35.086	56.345	-166.277	-93.950	8.555
2500	20.000	59.379	36.041	58.345	-166.006	-90.940	7.950
2600	20.000	60.164	36.954	60.345	-165.749	-87.942	7.392
2700	20.000	60.918	37.828	62.345	-165.507	-84.957	6.876
2741	20.000	61.220	38.175	63.165	-165.412	-83.734	6.676
2741	20.000	61.220	38.175	63.165	-171.812	-83.734	6.676
2800	20.000	61.646	38.665	64.345	-171.660	-81.837	6.387
2900	20.000	62.348	39.470	66.345	-171.4[illegible]	-78.634	5.926
3000	20.000	63.026	40.244	[illegible]8.345	-171.1[illegible]	-75.441	5.496
3100	20.000	63.681	40.989	70.345	-170.91[illegible]	-72.248	5.093
3200	20.000	64.316	41.709	72.345	-170.679	-69.077	4.717
3300	20.000	64.932	42.403	74.345	-170.444	-65.902	4.364
3400	20.000	65.529	43.074	76.345	-170.214	-62.734	4.032
3500	20.000	66.109	43.724	78.345	-169.988	-59.577	3.720
3600	20.000	66.672	44.354	80.345	-169.766	-56.428	3.425
3700	20.000	67.220	44.965	82.345	-169.547	-53.285	3.147
3800	20.000	67.753	45.557	84.345	-169.332	-50.140	2.884
3900	20.000	68.273	46.133	86.345	-169.121	-47.008	2.634
4000	20.000	68.779	46.693	88.345	-168.9[illegible]	-43.876	2.397
4100	20.000	69.273	47.238	90.345	-168.709	-40.755	2.172
4200	20.000	69.755	47.768	92.345	-168.509	-37.635	1.958
4300	20.000	70.226	48.285	94.345	-1[illegible]8.312	-34.519	1.754
4400	20.000	70.685	48.789	96.345	-168.120	-31.408	1.560
4500	20.000	71.135	49.280	98.345	-167.931	-[illegible]8.304	1.375
4600	20.000	71.574	49.760	0.345	-167.747	-25.198	1.197
4700	20.000	72.005	50.229	102.345	-167.568	-22.105	1.028
4800	20.000	72.426	50.687	104.345	-167.395	-19.008	0.865
4900	20.000	72.838	51.135	106.345	-167.228	-15.91[illegible]	0.710
5000	20.000	73.242	51.573	108.345	-167.069	-12.830	0.561
5031.58	20.000	73.368	51.710	108.977	-167.021	-11.921	0.518
5031.58	20.000	73.368	51.710	108.977	-329.594	-11.921	0.518
5100	20.000	73.638	52.002	110.345	-329.534	-7.600	0.326
5200	20.000	74.027	52.422	112.345	-329.461	-1.284	0.054
5300	20.000	74.407	52.833	114.345	-329.406	5.025	-0.207
5400	20.000	74.781	53.236	116.345	-329.371	11.339	-0.459
5500	20.000	75.148	53.631	118.345	-329.359	17.650	-0.701
5600	20.000	75.509	54.019	120.345	-329.373	23.955	-0.935
5700	20.000	75.863	54.399	127.345	-329.417	30.270	-1.161
5800	20.000	76.211	54.772	124.345	-329.497	36.592	-1.379
5900	20.000	76.552	55.138	126.345	-329.618	42.909	-1.589
6000	20.000	76.889	55.498	128.345	-329.787	49.230	-1.793

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$\Delta H^\circ_{f298.15} = -190.2$ kcal gfw^{-1}

$S^\circ_{298.15} = 13.03$ cal deg K^{-1}gfw^{-1}

$T_t = 1090$°K

$\Delta H_t = 0.720$ kcal gfw^{-1}

$T_t = 1200$°K

$\Delta H_t = 0$

$T_m = 2270$°K

$\Delta H_m = 15.0$ cal gfw^{-1}

$H^\circ_{298.15} - H^\circ_0 = 2.222$ kcal gfw^{-1}

$C^\circ_p = 11.70 + 9.56 \times 10^{-3}T - 0.72 \times 10^5 T^{-2}$ cal deg K^{-1} gfw^{-1} $298.15°K \leq T \leq 1090°K$

$C^\circ_p = 22.20$ cal deg K^{-1}gfw^{-1} $1090°K \leq T \leq 1200°K$

$C^\circ_p = 19.85$ cal deg K^{-1}gfw^{-1} $1200°K \leq T \leq 2270°K$

$C^\circ_p = 20.0$ cal deg K^{-1}gfw^{-1} $2270°K \leq T \leq 6000°K$

Structure

Brauer[1] reported that NbO_2 has a narrow range of homogeneity with a structure related to that of rutile. Other forms appear possible.

Heat of Formation

Three calorimetric determinations were recomputed.[2-4] See volume 1, this study (section IVB15.4.2) for details.

Heat Capacity and Entropy

Low temperature data from King.[5] Data from 298.15 to 1800°K from King and Christensen.[6] Data above 1800°K are estimated.

Melting and Vaporization

Melting temperature is average of two determinations.

References

1. Brauer, G., Z. Anorg. Chem. 248, 1-31 (1941).
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3. Kusenko, F.G. and P.V. Gel'd, Izv. Sibir Otd A. N.S.S.S.R. 1960, No. 2, 46-52 (1960).
4. Mah, A.D., J. Am. Chem. Soc 80, 3872 (1958).
5. King, E.G., J., Am. Chem. Soc. 80, 1799 (1958).
6. King, E.G. and A.U. Christensen, Bur Mines Rept 5789 (1961).

NIOBIUM DIOXIDE (NbO_2) (CONDENSED PHASE) GFW = 124.91

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw			Kcal/gfw			Log K_p
	C°_p	S°_T	$-(F^\circ_T - H^\circ_{298})/T$	$H^\circ_T - H^\circ_{298}$	ΔH°_f	ΔF°_f	
298.15	±0.200	±0.070	±0.070	±0.000	±1.000		
1000	±0.200	±0.312	±0.172	±0.140			
1090	±0.200	±0.329	±0.184	±0.158			
1090	±0.500	±0.421	±0.184	±0.258			
1200	±0.500	±0.469	±0.208	±0.313			
1200	±1.000	±0.552	±0.208	±0.413			
1500	±1.000	±0.776	±0.300	±0.713			
2000	±1.000	±1.063	±0.457	±1.213			
2270	±1.000	±1.190	±0.536	±1.483			
2270	±2.000	±3.393	±0.536	±6.483			
3000	±2.000	±3.950	±1.302	±7.943			
4000	±2.000	±4.526	±2.040	±9.943			
5000	±2.000	±4.972	±2.583	±11.943			
6000	±2.000	±5.336	±3.013	±13.943			

NIOBIUM DIOXIDE — IDEAL MOLECULAR GAS — **NbO_2**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Nb from 0° to 2741°K, Liquid Nb from 2741° to 5032°K, Gaseous Nb from 5032° to 6000°K; Gaseous O_2; Gaseous NbO_2.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.691	-50.403	-50.403	INFINITE
298.15	11.218	61.031	61.031	0.000	-51.051	-51.953	38.080
300	11.239	61.101	61.031	0.021	-51.054	-51.958	37.850
400	12.314	64.484	61.485	1.200	-51.185	-52.237	28.540
500	13.236	67.334	62.377	2.478	-51.247	-52.492	22.943
600	13.986	69.816	63.415	3.841	-51.259	-52.739	19.209
700	14.562	72.018	64.490	5.270	-51.235	-52.989	16.543
800	14.980	73.991	65.556	6.748	-51.193	-53.241	14.544
900	15.267	75.773	66.594	8.261	-51.142	-53.501	12.991
1000	15.452	77.392	67.594	9.798	-51.090	-53.765	11.750
1100	15.562	78.871	68.553	11.349	-51.045	-54.034	10.735
1200	15.619	80.227	69.470	12.909	-51.009	-54.308	9.890
1300	15.639	81.479	70.346	14.472	-50.989	-54.584	9.176
1400	15.636	82.638	71.183	16.036	-50.985	-54.860	8.564
1500	15.618	83.716	71.983	17.599	-50.997	-55.137	8.033
1600	15.591	84.723	72.748	19.159	-51.029	-55.413	7.569
1700	15.559	85.667	73.481	20.717	-51.078	-55.687	7.159
1800	15.524	86.556	74.183	22.271	-51.1[illegible]7	-55.956	6.794
1900	15.489	87.394	74.856	23.821	-51.235	-56.219	6.466
2000	15.454	88.188	75.503	25.369	-51.340	-56.477	6.171
2100	15.421	88.941	76.125	26.912	-51.466	-56.732	5.904
2200	15.390	89.657	76.724	28.453	-51.608	-56.980	5.660
2300	15.360	90.341	77.302	29.990	-51.769	-57.222	5.437
2400	15.332	90.994	77.859	31.525	-51.948	-57.457	5.232
2500	15.306	91.619	78.397	33.057	-52.145	-57.681	5.042
2600	15.282	92.219	78.917	34.586	-52.359	-57.897	4.866
2700	15.259	92.795	79.420	36.113	-52.590	-58.106	4.703
2741	15.251	93.025	79.622	36.739	-52.689	-58.191	4.640
2741	15.251	93.025	79.622	36.739	-59.089	-58.191	4.640
2800	15.238	93.350	79.908	37.638	-59.218	-58.169	4.540
2900	15.219	93.884	80.381	39.161	-59.443	-58.127	4.380
3000	15.201	94.400	80.839	40.682	-59.674	-58.077	4.231
3100	15.185	94.898	81.285	42.201	-59.912	-58.017	4.090
3200	15.170	95.380	81.718	43.719	-60.156	-57.957	3.958
3300	15.155	95.847	82.139	45.235	-60.405	-57.882	3.833
3400	15.142	96.299	82.549	46.750	-60.660	-57.800	3.715
3500	15.130	96.738	82.948	48.764	-60.9[illegible]	-57.712	3.603
3600	15.119	97.164	83.337	49.776	-61.186	-57.617	3.498
3700	15.108	97.578	83.716	51.287	-61.456	-57.515	3.397
3800	15.098	97.981	84.086	52.798	-61.730	-57.401	3.301
3900	15.089	98.373	84.448	54.307	-62.0[illegible]0	-57.287	3.210
4000	15.080	98.755	84.801	55.815	-62.294	-57.159	3.123
4100	15.072	99.127	85.146	57.323	-62.582	-57.029	3.040
4200	15.065	99.490	85.483	58.830	-62.875	-56.889	2.960
4300	15.058	99.844	85.813	60.336	-63.172	-56.740	2.884
4400	15.051	100.190	86.135	61.842	-63.474	-56.582	2.810
4500	15.045	100.529	86.452	63.346	-63.781	-56.428	2.740
4600	15.039	100.859	86.761	64.851	-64.092	-56.254	2.673
4700	15.034	101.183	87.065	66.354	-64.410	-56.085	2.608
4800	15.028	101.499	87.362	67.857	-64.734	-55.899	2.545
4900	15.023	101.809	87.654	69.360	-65.064	-55.711	2.485
5000	15.019	102.112	87.940	70.862	-65.403	-55.516	2.426
5031.58	15.017	102.207	88.029	[illegible] 336	-65.513	-55.514	2.411
5031.58	15.017	102.207	88.029	71.336	-228.086	-55.514	2.411
5100	15.015	102.410	88.221	72.364	-228.366	-53.167	2.278
5200	15.010	102.701	88.496	73.865	-228.792	-49.720	2.090
5300	15.006	102.987	88.767	75.366	-229.236	-46.276	1.908
5400	15.003	103.268	89.033	76.866	-229.701	-42.816	1.733
5500	14.999	103.543	89.294	78.3[illegible]6	-230.189	-39.347	1.563
5600	14.996	103.813	89.551	79.866	-230.703	-35.875	1.400
5700	14.993	104.078	89.804	81.365	-231.248	-32.389	1.242
5800	14.990	1[illegible]4.339	90.052	82.865	-231.828	-28.883	1.088
5900	14.987	104.595	90.296	84.363	-232.451	-25.374	0.940
6000	14.984	104.847	90.537	85.862	-233.121	-21.855	0.796

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NIOBIUM DIOXIDE (NbO_2) (IDEAL MOLECULAR GAS) gfw = 124.91

$\Delta H_{f0}^{\circ} = -50.403$ kcal gfw^{-1}

$\Delta H_{f298.15}^{\circ} = -51.051$ kcal gfw^{-1}

Point Group $D_{\infty h}$

$S_{298.15}^{\circ} = 61.031$ cal deg^{-1} gfw^{-1}

$H_{298.15}^{\circ} - H_0^{\circ} = 2.691$ kcal gfw^{-1}

Vibrational Levels and Multiplicities

ω, cm^{-1}	ω, cm^{-1}
913.6 (1)	1059.2 (1)
276.2 (2)	

Bond lengths and angles:

Nb-O distance = 1.691 A

O-Nb-O angle = 180°

Moment of inertia:

$I = 15.1918 \times 10^{-39}$ gm cm^2 $\sigma = 2$

$B_e = 0.18424$ cm^{-1}

Heat of Formation

Data of Shchukarev et al[1] was recalculated.

Heat Capacity and Entropy

Estimated structural data was used. Electronic levels were approximated as equal to those of Nb^{+4}.

Reference

1. Shchukarev, S. A., G. A. Semenov, and K. E. Frantseva, Doklady Akad. Nauk SSSR 145, 119 (1962).

NIOBIUM DIOXIDE (NbO_2) (IDEAL MOLECULAR GAS) GFW = 124.91

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^{\circ} - H_{298}^{\circ})/T$	$H_T^{\circ} - H_{298}^{\circ}$	ΔH_f°	ΔF_f°	log K_p
298.15	±1.000	±3.000	±3.000	±0.000	±5.000		
1000	±1.000	±4.210	±3.508	±0.702			
2000	±1.000	±4.903	±4.052	±1.702			
3000	±1.000	±5.309	±4.408	±2.702			
4000	±1.000	±5.596	±4.671	±3.702			
5000	±1.000	±5.820	±4.879	±4.702			
6000	±1.000	±6.002	±5.052	±5.702			

NIOBIUM PENTOXIDE CONDENSED PHASE Nb_2O_5

Reference State for Calculating ΔH_f°, ΔF_f°, and Log Kp: Solid Nb from 0° to 2741°K, Liquid Nb from 2741° to 5032°K, Gaseous Nb from 5032° to 6000°K, Gaseous O_2, Solid Nb_2O_5 from 0° to 1785°K, Liquid Nb_2O_5 from 1785° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-5.325	-452.210	-452.210	INFINITE
298.15	31.564	32.800	32.800	0.000	-454.600	-422.484	309.674
300	31.658	32.996	32.801	0.058	-454.596	-422.285	307.620
400	35.135	42.640	34.092	3.419	-454.210	-411.565	224.858
500	37.020	50.700	36.631	7.035	-453.640	-400.968	175.255
600	38.278	57.567	39.562	10.803	-453.000	-390.491	142.229
700	39.239	63.542	42.570	14.681	-452.320	-380.128	118.676
800	40.043	68.836	45.529	18.646	-451.626	-369.862	101.037
900	40.755	73.594	48.387	22.686	-450.917	-359.684	87.339
1000	41.410	77.922	51.127	26.795	-450.192	-349.583	76.398
1100	42.028	81.898	53.747	30.967	-449.452	-339.558	67.461
1200	42.620	85.581	56.248	35.199	-448.692	-329.601	60.026
1300	43.195	89.015	58.638	39.490	-447.915	-319.711	53.746
1400	43.757	92.237	60.924	43.838	-447.119	-309.878	48.372
1500	44.309	95.274	63.114	48.241	-446.301	-300.104	43.723
1600	44.854	98.152	65.214	52.700	-445.4[illegible]5	-290.385	39.663
1700	45.393	100.887	67.233	57.212	-444.608	-280.721	36.087
1785	45.848	103.113	68.889	61.090	-443.864	-272.541	33.367
1785	57.900	116.889	68.889	85.680	-419.274	-272.541	33.367
1800	57.900	117.373	69.291	86.548	-418.963	-271.312	32.940
1900	57.900	120.504	71.905	92.338	-416.896	-263.165	30.269
2000	57.900	123.474	74.409	98.128	-414.867	-255.120	27.877
2100	57.900	126.298	76.814	103.918	-412.863	-247.186	25.724
2200	57.900	128.992	79.125	109.708	-410.894	-239.344	23.776
2300	57.900	131.566	81.349	115.498	-408.958	-231.589	22.005
2400	57.900	134.030	83.493	121.288	-407.057	-223.920	20.390
2500	57.900	136.394	85.562	127.078	-405.189	-216.326	18.910
2600	57.900	138.664	87.561	132.868	-403.351	-208.805	17.551
2700	57.900	140.850	89.495	138.658	-401.546	-201.363	16.298
2741	57.900	141.722	90.269	141.032	-400.815	-198.330	15.813
2741	57.900	141.722	90.269	141.032	-413.615	-198.330	15.813
2800	57.900	142.955	91.367	144.448	-412.533	-193.704	15.119
2900	57.900	144.987	93.181	150.238	-410.713	-185.919	14.011
3000	57.900	146.950	94.941	156.028	-408.903	-178.203	12.981
3100	57.900	148.848	96.649	161.818	-407.1[illegible]	-170.530	12.022
3200	57.900	150.687	98.309	167.608	-405.321	-162.938	11.128
3300	57.900	152.468	99.923	173.398	-403.543	-155.386	10.290
3400	57.900	154.197	101.494	179.188	-401.778	-147.888	9.506
3500	57.900	155.875	103.024	184.978	-400.023	-140.445	8.769
3600	57.900	157.506	104.515	190.768	-398.278	-133.057	8.077
3700	57.900	159.093	105.969	196.558	-396.541	-125.718	7.426
3800	57.900	160.637	107.387	202.348	-394.813	-118.412	6.810
3900	57.900	162.141	108.772	208.138	-393.096	-111.164	6.229
4000	57.900	163.607	110.125	213.928	-391.386	-103.950	5.679
4100	57.900	165.036	111.447	219.718	-389.686	-96.789	5.159
4200	57.900	166.432	112.739	225.508	-387.996	-89.662	4.665
4300	57.900	167.794	114.004	231.298	-386.313	-82.573	4.197
4400	57.900	169.125	115.241	237.088	-384.643	-75.522	3.751
4500	57.900	170.426	116.453	242.878	-382.981	-68.523	3.328
4600	57.900	171.699	117.641	248.668	-381.331	-61.544	2.924
4700	57.900	172.944	118.804	254.458	-379.693	-54.411	2.539
4800	57.900	174.163	119.945	[illegible]	-378.071	-47.706	2.172
4900	57.900	175.357	121.063	[illegible]	-376.463	-40.832	1.821
5000	57.900	176.527	122.161	271.828	-374.876	-34.000	1.486
5031.58	57.900	176.891	122.503	273.657	-374.380	-31.970	1.389
5031.58	57.900	176.891	122.503	273.657	-699.526	-31.970	1.389
5100	57.900	177.673	123.238	277.618	-698.541	-22.900	0.981
5200	57.900	178.798	124.296	283.408	-697.135	-9.657	0.406
5300	57.900	179.900	125.335	289.198	-695.771	3.545	-0.146
5400	57.900	180.983	126.355	294.988	-694.455	16.739	-0.677
5500	57.900	182.045	127.358	300.778	-693.194	29.903	-1.188
5600	57.900	183.088	128.344	306.568	-691.995	43.036	-1.679
5700	57.900	184.113	129.314	312.358	-690.869	56.160	-2.153
5800	57.900	185.120	130.267	318.148	-689.831	69.282	-2.610
5900	57.900	186.110	131.205	323.938	-688.894	82.371	-3.051
6000	57.900	187.083	132.128	329.728	-688.074	95.456	-3.477

15 September 1963 HLS

NIOBIUM PENTOXIDE (Nb_2O_5) (CONDENSED PHASE) gfw = 265.82

$\Delta H^\circ_{f298.15}$ = -454.6 ± 1.0 kcal gfw^{-1} $S^\circ_{298.15}$ = 32.8 ± 0.2 cal deg K^{-1} gfw^{-1}

T_m = 1785°K ΔH_m = 24,590 kcal gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 5.325 kcal gfw^{-1}

$C^\circ_p = 36.90 + 5.12 \times 10^{-3}T - 6.10 \times 10^5 T^{-2}$ cal deg K^{-1} gfw^{-1} $298.15°K \leq T \leq 1785°K$

C°_p = 57.90 cal deg K^{-1} gfw^{-1} $1785°K \leq T \leq 6000°K$

Structure

The α-Nb_2O_5 (high temperature form) reported by Holtzberg[1] was considered to have a monoclinic unit cell.

Heat of Formation

Average of five calorimetric measurements.[2-6]

Heat Capacity and Entropy

Low temperature data from King.[7] High temperature data from Kelley.[8] Data above 1809°K were extrapolated.

Melting and Vaporization

Heat of melting was from Kelley[8] and Orr.[9]

References

1. Holtzberg, F. et al, J. Am. Chem. Soc. 79, 2039 (1957).
2. Humphrey, G. L., J. Am. Chem. Soc. 76, 978 (1954).
3. Morozova, M. P. and T. A. Stolyarova, Zhur Ob. Khim 30, 3848 (1960).
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8. Kelley, K. K., U.S. Bur. Mines Bull. 584 (1960).
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NIOBIUM PENTOXIDE (Nb_2O_5) (CONDENSED PHASE) GFW = 265.82

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw C°_p	S°_T	$-(F^\circ_T - H^\circ_{298})/T$	Kcal/gfw $H^\circ_T - H^\circ_{298}$	ΔH°_f	ΔF°_f	Log K_p
298.15	±0.300	±0.200	±0.200	±0.000	±1.000		
500	±0.300	±0.355	±0.234	±0.061			
500	±1.000	±0.355	±0.234	±0.061			
1000	±1.000	±1.048	±0.488	±0.561			
1785	±1.000	±1.628	±0.874	±1.346			
1785	±1.000	±2.188	±0.874	±2.346			
2000	±1.000	±2.302	±1.021	±2.561			
2000	±2.000	±2.302	±1.021	±2.561			
3000	±2.000	±3.113	±1.592	±4.561			
3000	±3.000	±3.113	±1.592	±4.561			
4000	±3.000	±3.976	±2.085	±7.561			
5000	±3.000	±4.645	±2.533	±10.561			
6000	±3.000	±5.192	±2.932	±13.561			

TABLE 180

OXYGEN

IDEAL MONATOMIC GAS

O

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p:
Gaseous O_2 from 0° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	[illegible].000	INFINITE	-1.608	58.986	58.986	INFINITE
298.15	5.237	38.469	38.469	0.000	59.557	55.393	-40.602
300	5.235	38.501	38.469	0.010	59.561	55.367	-40.333
400	5.135	39.992	38.673	0.528	59.724	53.945	-29.473
500	5.081	41.131	39.055	1.038	59.868	52.483	-22.939
600	5.049	42.054	39.480	1.544	59.996	50.994	-18.547
700	5.029	42.831	39.905	2.048	60.111	49.484	-15.449
800	5.015	43.502	40.314	2.550	60.214	47.959	-13.101
900	5.006	44.092	40.701	3.052	60.309	46.421	-11.272
1000	4.999	44.619	41.067	3.552	60.395	44.873	-9.806
1100	4.994	45.095	41.412	4.051	60.475	43.317	-8.606
1200	4.990	45.529	41.737	4.551	60.550	41.754	-7.604
1300	4.987	45.929	42.045	5.049	60.621	40.184	-6.755
1400	4.984	46.298	42.335	5.548	60.688	38.610	-6.027
1500	4.982	46.642	42.611	6.046	60.750	37.031	-5.395
1600	4.981	46.963	42.873	6.544	60.810	35.448	-4.842
1700	4.979	47.265	43.123	7.042	60.866	33.860	-4.353
1800	4.979	47.550	43.361	7.540	60.920	32.271	-3.918
1900	4.978	47.819	43.588	8.038	60.971	30.679	-3.529
2000	4.978	47.074	43.806	8.536	61.019	29.083	-3.178
2100	4.978	48.317	44.016	9.034	61.064	27.484	-2.860
2200	4.979	48.549	44.216	9.532	61.107	25.884	-2.571
2300	4.980	48.770	44.410	10.029	61.145	24.282	-2.307
2400	4.981	48.982	44.596	10.527	61.182	22.679	-2.065
2500	4.984	49.186	44.775	11.026	61.218	21.075	-1.842
2600	4.986	49.381	44.949	11.524	61.249	19.468	-1.636
2700	4.990	59.569	45.116	12.023	61.280	17.861	-1.446
2800	4.994	49.751	42.279	12.522	61.307	16.249	-1.268
2900	4.999	49.926	45.436	13.022	61.334	14.642	-1.103
3000	5.004	50.096	45.588	13.[illegible]22	61.357	13.033	-0.949
3100	5.010	50.260	45.736	14.023	61.380	11.420	-0.805
3200	5.017	50.419	45.880	14.524	61.400	9.810	-0.670
3300	5.025	50.574	46.020	15.026	61.419	8.196	-0.543
3400	5.033	50.724	46.156	15.529	61.438	6.585	-0.423
3500	5.041	50.870	46.289	16.033	61.455	4.967	-0.310
3600	5.050	51.012	46.418	16.537	61.470	3.354	-0.204
3700	5.060	51.150	46.544	17.043	61.485	1.741	-0.103
3800	5.070	51.285	46.667	17.549	61.498	0.125	-0.007
3900	5.081	51.417	46.787	18.057	61.512	-1.490	0.083
4000	5.091	51.546	46.905	18.565	61.524	-3.107	0.170
4100	5.103	51.672	47.019	19.075	61.536	-4.719	0.252
4200	5.114	51.795	47.132	19.586	61.547	-6.337	0.330
4300	5.126	51.916	47.242	20.098	61.557	-7.953	0.404
4400	5.138	52.033	47.349	20.611	61.567	-9.567	0.475
4500	5.150	52.149	47.455	21.126	61.576	-11.188	0.543
4600	5.162	52.262	47.558	21.641	61.583	-12.801	0.608
4700	5.174	52.374	47.659	22.158	61.589	-14.416	0.670
4800	5.186	52.483	47.758	22.676	61.594	-16.033	0.730
4900	5.198	52.590	47.856	23.195	61.596	-17.652	0.787
5000	5.210	52.695	47.952	23.715	61.596	-19.268	0.842
5100	5.222	52.798	48.046	24.237	61.593	-20.885	0.895
5200	5.234	52.900	48.138	24.760	61.586	-22.499	0.946
5300	5.246	52.999	48.229	25.284	61.574	-24.114	0.994
5400	5.258	53.098	48.318	25.[illegible]09	61.555	-25.731	1.041
5500	5.269	53.194	48.406	26.335	61.528	-27.348	1.087
5600	5.280	53.289	48.492	26.863	61.493	-28.957	1.130
5700	5.292	53.383	48.577	27.392	61.445	-30.571	1.172
5800	5.302	53.475	48.661	27.921	61.383	-32.182	1.213
5900	5.313	53.566	48.743	28.452	61.303	-33.793	1.252
6000	5.323	53.655	48.824	28.984	61.202	-35.399	1.289

May 1962 RCF

OXYGEN, MONATOMIC (O) (IDEAL GAS) gfw = 16.000

ΔH^o_{f0} = 58.986 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 59.557 kcal gfw^{-1}

Ground State Configuration = $^3P_2$

$S^o_{298.15}$ = 38.469 cal degK^{-1}gfw^{-1}

$H^o_{298.15} - H^o_0$ = 1.608 kcal gfw^{-1}

Electronic Levels and Multiplicities

Energy levels from Moore.[1]

Heat of Formation

Dissociation energy from Brix and Herzberg.[2]

Heat Capacity and Entropy

Calculated on monatomic gas-computer program.

See Barriault *et al*[3] for further details.

References

1. Moore, C. Atomic Energy Levels, Vol. 1, Nat. Bur. Stds. (1949).
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3. Barriault, R. J. *et al*, ASD TR 61-260 (May 1962), Pt. 1.

OXYGEN, MONATOMIC (O) (IDEAL GAS) GFW = 16.000

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw			Kcal gfw			
	C_p^o	S_T^o	$-(F_T^o - H_{298}^o)/T$	$H_T^o - H_{298}^o$	ΔH_f	ΔF_f	Log K_p
298.15	±0.000	±0.002	±0.002	±0.000	±0.020	±0.021	±0.015
1000	±0.000	±0.002	±0.002	±0.000	±0.021	±0.024	±0.005
2000	±0.000	±0.002	±0.002	±0.000	±0.022	±0.028	±0.003
3000	±0.000	±0.002	±0.002	±0.000	±0.025	±0.032	±0.002
4000	±0.000	±0.002	±0.003	±0.001	±0.035	±0.044	±0.002
5000	±0.000	±0.002	±0.003	±0.001	±0.078	±0.053	±0.002
6000	±0.000	±0.002	±0.003	±0.001	±0.428	±0.077	±0.003

TABLE 181

OSMIUM MONOXIDE IDEAL MOLECULAR GAS **OOs**

Reference State for Calculating ΔH_f°, ΔF_f° and Log K_p: Solid Os from 0° to 3290°K, Liquid Os from 3290° to 5270°K, Gaseous Os from 5270° to 6000°K; Gaseous O_2; Gaseous OsO.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.124	102.123	102.123	INFINITE
298.15	7.614	60.396	60.396	0.000	102.000	93.624	-68.625
300	7.623	60.433	60.396	0.014	101.997	93.572	-68.164
400	8.003	62.691	60.700	0.796	101.873	90.791	-49.603
500	8.263	64.507	61.286	1.611	101.665	88.051	-38.485
600	8.436	66.030	61.953	2.446	101.504	85.343	-31.085
700	8.554	67.340	62.631	3.296	101.339	82.663	-25.807
800	8.636	68.488	63.293	4.156	101.166	80.006	-21.856
900	8.695	69.509	63.948	5.022	100.981	77.372	-18.788
1000	8.739	70.427	64.533	5.894	100.787	74.760	-16.338
1100	8.773	71.262	65.107	6.770	100.581	72.167	-14.338
1200	8.799	72.026	65.652	7.649	100.366	69.593	-12.674
1300	8.819	72.731	66.170	8.530	100.139	67.037	-11.269
1400	8.836	73.386	66.662	9.417	99.901	64.501	-10.069
1500	8.849	73.996	67.131	10.297	99.656	61.981	-9.030
1600	8.860	74.567	67.578	11.182	99.396	59.476	-8.124
1700	8.869	75.105	68.005	12.069	99.137	56.991	-7.326
1800	8.877	75.612	68.414	12.956	98.847	54.519	-6.619
1900	8.884	76.092	68.806	13.844	98.556	52.063	-5.988
2000	8.889	76.548	69.181	14.733	98.255	49.626	-5.423
2100	8.894	76.982	69.543	15.622	97.941	47.202	-4.912
2200	8.899	77.395	69.890	16.511	97.616	44.794	-4.450
2300	8.902	77.791	70.225	17.402	97.283	42.399	-4.029
2400	8.905	78.170	70.548	18.292	96.936	40.021	-3.644
2500	8.908	78.534	70.861	19.183	96.579	37.654	-3.292
2600	8.911	78.883	71.162	20.074	96.210	35.309	-2.968
2700	8.913	79.219	71.455	20.965	95.830	32.970	-2.669
2800	8.915	79.544	71.738	21.856	95.439	30.650	-2.392
2900	8.917	79.856	72.012	22.748	95.037	28.344	-2.136
3000	8.919	80.159	72.279	23.640	94.625	26.051	-1.898
3100	8.920	80.451	72.538	24.532	94.200	23.773	-1.676
3200	8.922	80.734	72.790	25.424	93.765	21.506	-1.469
3290	8.923	80.982	73.010	26.227	93.364	19.482	-1.294
3290	8.923	80.982	73.010	26.227	85.798	19.482	-1.294
3300	8.923	81.009	73.034	26.316	85.749	19.282	-1.277
3400	8.924	81.275	73.273	27.208	85.2[illegible]	17.274	-1.110
3500	8.925	81.534	73.505	28.101	84.762	15.282	-0.954
3600	8.926	81.786	73.732	28.993	84.265	13.301	-0.807
3700	8.927	82.030	73.953	29.886	83.767	11.339	-0.670
3800	8.928	82.268	74.169	30.779	83.268	9.388	-0.540
3900	8.928	82.500	74.379	31.671	82.765	7.450	-0.417
4000	8.929	82.726	74.585	32.564	82.262	5.526	-0.302
4100	8.930	82.947	74.786	33.457	81.757	3.616	-0.193
4200	8.930	83.162	74.983	34.350	81.250	1.717	-0.089
4300	8.931	83.372	75.176	35.243	80.742	-0.172	0.009
4400	8.932	83.577	75.364	36.137	80.232	-2.047	0.102
4500	8.932	83.778	75.549	37.030	79.719	-3.912	0.190
4600	8.932	83.974	75.730	37.923	79.204	-5.760	0.274
4700	8.933	84.166	75.908	38.816	78.695	-7.604	0.354
4800	8.933	84.355	76.082	39.709	78.160	-9.434	0.430
4900	8.934	84.539	76.252	40.603	77.644	-11.251	0.502
5000	8.934	84.719	76.420	41.496	77.116	-13.060	0.571
5100	8.934	84.896	76.584	42.390	76.585	-14.856	0.637
5200	8.935	85.070	76.746	43.283	76.048	-16.643	0.699
5269.57	8.935	85.189	76.857	43.909	75.672	-17.895	0.742
5269.57	8.935	85.189	76.857	43.909	-100.729	-17.895	0.742
5300	8.935	85.240	76.905	44.177	-100.889	-17.401	0.718
5400	8.935	85.407	77.061	45.070	-101.419	-15.817	0.640
5500	8.936	85.571	77.214	45.964	-101.960	-14.388	0.572
5600	8.936	85.732	77.364	46.857	-102.516	-12.624	0.493
5700	8.936	85.890	77.513	47.751	-103.086	-11.014	0.422
5800	8.936	86.045	77.658	48.644	-103.676	-9.386	0.354
5900	8.936	86.198	77.802	49.538	-104.285	-7.752	0.287
6000	8.937	86.348	77.943	50.431	-104.919	-6.108	0.222

15 September 1962 RCF

ΔH^o_{f0} = 102.123 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 102.000 kcal gfw^{-1}

Ground State Degenercy = 6

$S^o_{298.15}$ = 60.396 cal deg K^{-1}gfw^{-1}

$H^o_{298.15}-H^o_0$ = 2.124 kcal gfw^{-1}

		cm^{-1}							
State	g	E	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e \times 10^5$	$D_e \times 10^6$
X	6	0.0	795	3.6	---	0.34	0.0019	---	0.24

Heat of Formation

Value estimated. See volume 1, this study (section IVB18.4.1) for details.

Heat Capacity and Entropy

Spectroscopic constants from Brewer et al[1] used.

Reference

1. Brewer, L. and M. S. Chandrasekharaiah, U. S. At. Energy Comm. Rept. UCRL-8713 Rev. (June 1960).

TABLE 182

PLATINUM MONOXIDE — **IDEAL MOLECULAR GAS** — **OPt**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Pt from 0° to 2043°K, Liquid Pt from 2043° to 4108°K, Gaseous Pt from 4108° to 6000°K; Gaseous O_2; Gaseous PtO.

T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
	cal/°K gfw			Kcal/gfw			
0	0.000	0.000	INFINITE	-2.125	88.797	88.797	INFINITE
298.15	7.631	60.495	60.495	0.000	88.600	80.836	-59.251
300	7.639	60.543	60.496	0.014	88.597	80.787	-58.851
400	8.019	62.795	60.800	0.798	88.399	78.215	-42.733
500	8.276	64.614	61.387	1.614	88.209	75.691	-33.083
600	8.447	66.140	62.055	2.451	88.015	73.206	-26.664
700	8.562	67.451	62.735	3.301	87.813	70.753	-22.089
800	8.643	68.600	63.397	4.162	87.599	68.331	-18.666
900	8.701	69.621	64.033	5.029	87.370	65.936	-16.011
1000	8.744	70.540	64.639	5.902	87.127	63.567	-13.892
1100	8.777	71.375	65.214	6.778	86.869	61.223	-12.163
1200	8.802	72.140	65.760	7.657	86.598	58.903	-10.727
1300	8.822	72.846	66.278	8.538	86.312	56.606	-9.516
1400	8.838	73.500	66.771	9.421	86.012	54.332	-8.481
1500	8.851	74.110	67.240	10.306	85.697	52.082	-7.588
1600	8.862	74.682	67.687	11.191	85.367	49.852	-6.809
1700	8.871	75.219	68.115	12.078	85.024	47.640	-6.124
1800	8.879	75.727	68.524	12.965	84.664	45.453	-5.518
1900	8.885	76.207	68.916	13.854	8[illegible].292	43.284	-4.979
2000	8.891	76.663	69.292	14.742	83.903	41.136	-4.495
2043	8.893	76.852	69.447	15.125	83.732	40.276	-4.308
2043	8.893	76.852	69.447	15.125	79.034	40.276	-4.308
2100	8.895	77.097	69.653	15.632	78.797	39.140	-4.073
2200	8.900	77.511	70.001	16.521	78.381	37.260	-3.701
2300	8.903	77.906	70.336	17.412	77.964	35.400	-3.364
2400	8.906	78.285	70.659	18.302	77.543	33.560	-3.056
2500	8.909	78.649	70.972	19.193	77.120	31.734	-2.774
2600	8.912	78.998	71.274	20.084	76.695	29.927	-2.515
2700	8.914	79.335	71.566	20.975	76.267	28.138	-2.277
2800	8.916	79.659	71.849	21.867	75.838	26.364	-2.058
2900	8.918	79.972	72.124	22.758	75.405	24.604	-1.854
3000	8.919	80.274	72.391	23.650	74.971	22.859	-1.665
3100	8.921	80.567	72.650	24.542	74.534	21.130	-1.490
3200	8.922	80.850	72.902	25.434	74.095	19.414	-1.326
3300	8.923	81.12[illegible]	73.147	26.327	73.655	17.713	-1.173
3400	8.924	81.391	73.385	27.219	73.213	16.025	-1.030
3500	8.926	81.650	73.618	28.112	72.769	14.349	-0.896
3600	8.926	81.901	73.844	29.004	72.[illegible]	12.689	-0.770
3700	8.927	82.146	74.065	29.897	71.[illegible]	11.037	-0.652
3800	8.928	82.384	74.281	30.790	71.425	9.398	-0.541
3900	8.929	82.616	74.492	31.683	70.973	7.771	-0.435
4000	8.930	82.842	74.698	32.575	7[illegible].519	6.158	-0.336
4100	8.930	83.062	74.899	33.468	70.064	4.554	-0.243
4108.34	8.930	83.079	74.915	33.539	70.024	4.639	-0.247
4108.34	8.930	83.079	74.915	33.539	-51.495	4.639	-0.247
4200	8.931	83.277	75.096	34.361	-51.667	5.671	-0.295
4300	8.931	83.488	75.289	35.255	-51.861	7.038	-0.358
4400	8.932	83.693	75.478	36.148	-52.060	8.410	-0.418
4500	8.932	83.894	75.662	37.041	-52.264	9.792	-0.476
4600	8.933	84.090	75.843	37.934	-52.471	11.173	-0.531
4700	8.933	84.282	76.021	38.927	-52.684	12.559	-0.584
4800	8.934	84.470	76.195	39.721	-52.901	13.948	-0.635
4900	8.934	84.654	76.366	40.614	-53.123	15.343	-0.684
5000	8.934	84.835	76.533	41.508	-53.351	16.745	-0.732
5100	8.935	85.012	76.698	42.401	-53.587	18.144	-0.777
5200	8.935	85.185	76.859	43.294	-53.829	19.560	-0.822
5300	8.935	85.356	77.018	44.188	-54.080	20.975	-0.865
5400	8.935	85.523	77.174	45.082	-54.340	22.396	-0.906
5500	8.936	85.686	77.327	45.975	-54.611	23.818	-0.946
5600	8.936	85.847	77.478	46.869	-54.895	25.250	-0.985
5700	8.936	86.006	77.626	47.762	-55.195	26.687	-1.023
5800	8.936	86.161	77.772	48.656	-55.512	28.126	-1.060
5900	8.937	86.314	77.916	49.550	-55.850	29.571	-1.095
6000	8.937	86.464	78.057	50.443	-56.213	31.030	-1.130

15 December 1962 — RCF

PLATINUM MONOXIDE (PtO) (IDEAL MOLECULAR GAS) gfw = 211.09

ΔH^{o}_{f0} = 88.797 kcal gfw^{-1}

$\Delta H^{o}_{f298.15}$ = 88.600 kcal gfw^{-1}

Ground State Degeneracy = 6

$S^{o}_{298.15}$ = 60.495 cal deg K^{-1}gfw^{-1}

$H^{o}_{298.15}-H^{o}_{0}$ = 2.125 kcal gfw^{-1}

		cm^{-1}							
State	g	E	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e \times 10^5$	$D_e \times 10^6$
X	6	0	785	—	—	0.334	—	—	—

Heat of Formation

Estimated by analogy to data for PtO_2.

Heat Capacity and Entropy

Calculated using above estimated constants. See volume 1, this study (section IVB20.4.1) for details.

RHENIUM MONOXIDE **IDEAL MOLECULAR GAS** **ORe**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Re from 0° to 3453°K, Liquid Re from 3453° to 5960°K, Gaseous Re from 5960° to 6000°K; Gaseous O_2; Gaseous ReO.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.113	90.231	90.231	INFINITE
298.15	7.515	59.382	59.382	0.000	90.000	82.250	-60.288
300	7.523	59.429	59.382	0.014	89.996	82.202	-59.881
400	7.905	61.647	59.682	0.786	89.791	79.636	-43.509
500	8.180	63.443	60.260	1.591	89.600	77.119	-33.707
600	8.368	64.952	60.920	2.419	89.408	74.640	-27.186
700	8.499	66.252	61.591	3.263	89.212	72.195	-22.539
800	8.591	67.393	62.246	4.118	89.004	69.778	-19.062
900	8.658	68.409	62.876	4.980	88.782	67.387	-16.363
1000	8.708	69.324	63.476	5.849	88.550	65.023	-14.210
1100	8.747	70.156	64.046	6.722	88.304	62.682	-12.453
1200	8.776	70.919	64.587	7.598	88.043	60.364	-10.993
1300	8.800	71.622	65.102	8.477	87.768	58.067	-9.762
1400	8.819	72.275	65.591	9.358	87.479	55.795	-8.710
1500	8.834	72.884	66.057	10.240	87.173	53.542	-7.801
1600	8.847	73.455	66.502	11.124	86.852	51.310	-7.008
1700	8.858	73.991	66.927	12.010	96.515	49.098	-6.312
1800	8.867	74.498	67.333	12.896	86.161	46.909	-5.695
1900	8.874	74.977	67.723	13.783	85.790	44.739	-5.146
2000	8.881	75.433	68.097	14.671	85.40[illegible]	42.588	-4.654
2100	8.886	75.866	68.457	15.559	84.994	40.458	-4.210
2200	8.891	76.280	68.803	16.448	84.570	38.347	-3.809
2300	8.896	76.675	69.137	17.337	84.125	36.255	-3.445
2400	8.899	77.054	69.459	18.227	83.663	34.184	-3.113
2500	8.903	77.417	69.770	19.117	83.180	32.131	-2.809
2600	8.906	77.766	70.071	20.008	82.678	30.100	-2.530
2700	8.908	78.102	70.362	20.898	82.154	28.088	-2.273
2800	8.911	78.426	70.645	21.789	81.611	26.093	-2.037
2900	8.913	78.739	70.918	22.680	81.046	24.122	-1.818
3000	8.915	79.041	71.184	23.572	80.462	22.168	-1.615
3100	8.917	79.334	71.442	24.463	79.853	20.239	-1.427
3200	8.918	79.617	71.693	25.355	79.224	18.325	-1.251
3300	8.920	79.891	71.938	26.247	78.575	16.430	-1.088
3400	8.921	80.158	72.175	27.139	77.901	14.559	-0.936
3453	8.922	80.296	72.299	27.612	77.535	13.575	-0.859
3453	8.922	80.296	72.299	27.612	69.592	13.575	-0.859
3500	8.922	80.416	72.407	28.031	69.[illegible]	12.813	-0.800
3600	8.923	80.668	72.633	28.924	68.5[illegible]	11.209	-0.680
3700	8.924	80.912	72.854	29.816	67.87[illegible]	9.625	-0.568
3800	8.925	81.150	73.069	30.708	67.171	8.063	-0.464
3900	8.926	81.382	73.279	31.601	66.469	6.515	-0.365
4000	8.927	81.608	73.484	32.494	65.766	4.990	-0.273
4100	8.928	81.828	73.[illegible]85	33.[illegible]86	65.060	3.478	-0.185
4200	8.928	82.043	73.882	34.279	64.353	1.985	-0.103
4300	8.929	82.254	74.074	35.172	63.645	0.508	-0.026
4400	8.930	82.459	74.262	36.065	62.934	-0.952	0.047
4500	8.930	82.660	74.447	36.958	62.221	-2.399	0.116
4600	8.931	82.856	74.627	37.851	61.506	-3.822	0.182
4700	8.931	83.048	74.804	38.744	60.789	-5.231	0.243
4800	8.932	83.236	74.978	39.637	60.068	-6.631	0.302
4900	8.932	83.420	75.149	40.530	[illegible]	-8.012	0.357
5000	8.933	83.601	75.316	41.424	58.618	-9.380	0.410
5100	8.933	83.777	75.480	42.317	57.886	-10.730	0.460
5200	8.933	83.951	75.641	43.210	57.149	-12.066	0.507
5300	8.934	84.121	75.800	44.104	56.407	-13.395	0.552
5400	8.934	84.288	75.955	44.997	55.656	-14.701	0.595
5500	8.934	84.452	76.108	45.890	54.896	-15.993	0.635
5600	8.935	84.613	76.259	46.784	54.127	-17.276	0.674
5700	8.935	84.771	76.407	47.677	53.344	-18.545	0.711
5800	8.935	84.927	76.552	48.571	52.546	-19.791	0.746
5900	8.935	85.079	76.695	49.464	51.728	-21.026	0.779
5960.67	8.936	85.169	76.780	50.000	51.219	-21.762	0.798
5960.67	8.936	85.169	76.780	50.000	-117.096	-21.762	0.798
6000	8.936	85.229	76.836	50.358	-117.511	-21.132	0.770

15 December 1962 RCF

RHENIUM MONOXIDE (ReO) (IDEAL MOLECULAR GAS) gfw = 202.22

ΔH^o_{f0} = 90.231 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 90.000 kcal gfw^{-1}

Ground State Degeneracy = 4

$S^o_{298.15}$ = 59.382 cal deg K^{-1}gfw^{-1}

$H^o_{298.15}-H^o_0$ = 2.113 kcal gfw^{-1}

State	g	E (cm^{-1})	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e x10^5$	$D_e x10^6$
X	4	0	858	—	—	0.355	—	—	—

Heat of Formation

Estimated by comparison with neighboring elements in periodic table.

Heat Capacity and Entropy

Calculated using above estimated spectroscopic constants. See volume 1, this study (section IVB21.4.1) for details.

TABLE 184

RHODIUM MONOXIDE — **IDEAL MOLECULAR GAS** — **ORh**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Rh from 0° to 2239°K, Liquid Rh from 2239° to 3996°K, Gaseous Rh from 3996° to 6000°K; Gaseous O_2; Gaseous RhO.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.119	88.691	88.691	INFINITE
298.15	7.575	57.727	57.727	0.000	88.400	80.739	-59.181
300	7.583	57.774	57.727	0.014	88.396	80.692	-58.781
400	7.965	60.011	58.030	0.792	88.209	78.152	-42.698
500	8.231	61.819	58.613	1.603	88.015	75.659	-33.069
600	8.411	63.336	59.277	2.436	87.806	73.208	-26.665
700	8.533	64.643	59.952	3.283	87.578	70.793	-22.101
800	8.619	65.788	60.612	4.141	87.330	68.412	-18.688
900	8.682	66.807	61.244	5.006	87.060	66.063	-16.042
1000	8.728	67.724	61.847	5.877	86.768	63.745	-13.931
1100	8.763	68.558	62.420	6.752	86.453	61.458	-12.210
1200	8.790	69.322	62.964	7.629	86.116	59.201	-10.781
1300	8.812	70.026	63.480	8.509	85.756	56.972	-9.577
1400	8.829	70.680	63.971	9.392	85.376	54.772	-8.550
1500	8.844	71.289	64.439	10.275	84.972	52.600	-7.663
1600	8.855	71.861	64.885	11.160	84.547	50.455	-6.892
1700	8.865	72.398	65.312	12.046	84.099	48.338	-6.214
1800	8.873	72.905	65.720	12.933	83.628	46.247	-5.615
1900	8.880	73.385	66.110	13.821	83.136	44.186	-5.082
2000	8.886	73.840	66.486	14.709	82.621	42.148	-4.605
2100	8.891	74.274	66.846	15.598	82.083	40.139	-4.177
2200	8.896	74.688	67.193	16.487	81.523	38.155	-3.790
2239	8.898	74.843	67.324	16.834	81.299	37.389	-3.649
2239	8.898	74.843	67.324	16.834	76.149	37.389	-3.649
2300	8.900	75.083	67.528	17.377	75.803	36.334	-3.452
2400	8.903	75.462	67.851	18.267	75.231	34.629	-3.153
2500	8.906	75.826	68.162	19.158	74.659	32.951	-2.880
2600	8.909	76.175	68.464	20.049	74.083	31.295	-2.630
2700	8.911	76.511	68.756	20.940	73.506	29.657	-2.400
2800	8.914	76.835	69.039	21.831	72.925	28.046	-2.189
2900	8.916	77.148	69.313	22.722	72.342	26.455	-1.994
3000	8.917	77.450	69.579	23.614	71.758	24.882	-1.813
3100	8.919	77.743	69.838	24.506	71.172	23.329	-1.645
3200	8.920	78.026	70.089	25.398	70.583	21.797	-1.489
3300	8.922	78.301	70.334	26.290	69.993	20.278	-1.343
3400	8.923	78.567	70.572	27.182	69.399	18.783	-1.207
3500	8.924	78.826	70.804	28.074	68.[illegible]	17.303	-1.080
3600	8.925	79.077	71.031	28.967	68.208	15.840	-0.962
3700	8.926	79.322	71.251	29.859	67.610	14.396	-0.850
3800	8.927	79.560	71.467	30.752	6[illegible].010	12.964	-0.746
3900	8.928	79.791	71.677	31.645	66.409	11.552	-0.647
3995.89	8.928	80.008	71.875	32.502	65.826	10.206	-0.558
3995.89	8.928	80.008	71.875	32.502	-52.319	10.206	-0.558
4000	8.928	80.017	71.883	32.538	-52.327	10.258	-0.560
4100	8.929	80.238	72.084	33.430	-52.610	11.824	-0.630
4200	8.930	80.453	72.281	34.323	-52.895	13.405	-0.697
4300	8.930	80.663	72.473	35.216	-53.184	14.990	-0.762
4400	8.931	80.869	72.662	36.109	-53.477	16.574	-0.823
4500	8.931	81.069	72.846	37.003	-53.771	18.173	-0.883
4600	8.932	81.266	73.027	37.896	-54.071	19.777	-0.940
4700	8.932	81.458	73.205	38.789	-54.375	21.378	-0.994
4800	8.933	81.646	73.379	39.682	-54.683	22.998	-1.047
4900	8.933	81.830	73.549	40.575	-54.995	24.624	-1.098
5000	8.933	82.010	73.717	41.469	-55.313	26.250	-1.147
5100	8.934	82.187	73.881	42.362	-55.638	27.883	-1.195
5200	8.934	82.361	74.042	43.256	-55.969	29.531	-1.241
5300	8.935	82.531	74.201	44.149	-56.309	31.179	-1.286
5400	8.935	82.698	74.357	45.042	-56.658	32.829	-1.329
5500	8.935	82.862	74.510	45.936	-57.016	34.497	-1.371
5600	8.935	83.023	74.661	46.829	-57.390	36.155	-1.411
5700	8.936	83.181	74.809	47.723	-57.776	37.835	-1.451
5800	8.936	83.337	74.954	48.617	-58.180	39.520	-1.489
5900	8.936	83.489	75.098	49.510	-58.605	41.212	-1.527
6000	8.936	83.639	75.239	50.404	-59.054	42.908	-1.563

15 December 1962 — RCF

RHODIUM MONOXIDE (RhO) (IDEAL MOLECULAR GAS) gfw = 118.91

ΔH^{o}_{f0} = 88.691 kcal gfw^{-1}

$\Delta H^{o}_{f298.15}$ = 88.400 kcal gfw^{-1}

Ground State Degeneracy = 4

$S^{o}_{298.15}$ = 57.727 cal deg K^{-1}gfw^{-1}

$H^{o}_{298.15} - H^{o}_{0}$ = 2.119 kcal gfw^{-1}

		cm^{-1}							
State	g	E	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e \times 10^5$	$D_e \times 10^6$
X	4	0	820	—	—	0.373	—	—	—

Heat of Formation

Estimated by analogy to data for $RhO_{2(g)}$.

Heat Capacity and Entropy

Calculated using above estimated spectroscopic constants.

SILICON MONOXIDE — IDEAL MOLECULAR GAS — OSi

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Si from 0° to 1690°K, Liquid Si from 1690° to 3566°K, Gaseous Si from 3566° to 6000°K; Gaseous O_2, Gaseous SiO.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.083	-24.316	-24.316	INFINITE
298.15	7.146	50.544	50.544	0.000	-24.040	-30.453	22.322
300	7.151	50.588	50.544	0.013	-24.042	-30.493	22.213
400	7.442	52.684	50.828	0.742	-24.176	-32.624	17.824
500	7.736	54.377	51.374	1.502	-24.331	-34.719	15.175
600	7.983	55.810	51.997	2.288	-24.497	-36.781	13.397
700	8.178	57.056	52.632	3.096	-24.668	-38.814	12.118
800	8.329	58.158	53.256	3.922	-24.846	-40.824	11.152
900	8.447	59.146	53.856	4.761	-25.031	-42.810	10.395
1000	8.539	60.041	54.431	5.611	-25.224	-44.774	9.785
1100	8.613	60.859	54.978	6.468	-25.426	-46.719	9.282
1200	8.673	61.611	55.500	7.333	-25.634	-48.647	8.859
1300	8.723	62.307	55.997	8.203	-25.850	-50.555	8.499
1400	8.764	62.955	56.472	9.077	-26.075	-52.449	8.187
1500	8.799	63.561	56.924	9.955	-26.309	-54.323	7.914
1600	8.829	64.130	57.357	10.837	-26 551	-56.183	7.674
1690	8.853	64.614	57.731	11.633	-26.776	-57.845	7.480
1690	8.853	64.614	57.731	11.633	-38.726	-57.845	7.480
1700	8.855	64.666	57.771	11.721	-38.751	-57.957	7.450
1800	8.878	65.173	58.169	12.608	-39.012	-59.080	7.173
1900	8.899	65.653	58.550	13.497	-39.281	-60.187	6.923
2000	8.918	66.110	58.917	14.388	-39.557	-61.280	6.696
2100	8.934	66.546	59.270	15.280	-39.833	-62.360	6.490
2200	8.950	66.962	59.610	16.174	-40.110	-63.425	6.300
2300	8.964	67.360	59.938	17.070	-40.387	-64.480	6.127
2400	8.977	67.742	60.256	17.967	-40.668	-65.523	5.966
2500	8.990	68.109	60.562	18.865	-40.949	-66.551	5.818
2600	9.001	68.462	60.860	19.765	-41.230	-67.570	5.680
2700	9.012	68.801	61.148	20.666	-41.513	-68.581	5.551
2800	9.023	69.129	61.427	21.567	-41.799	-69.576	5.430
2900	9.033	69.446	61.698	22.470	-42.085	-70.563	5.318
3000	9.043	69.753	61.961	23.374	-42.373	-71.538	5.211
3100	9.053	70.050	62.218	24.279	-42.662	-72.507	5.111
3200	9.063	70.337	62.467	25.185	-42.953	-73.466	5.017
3300	9.072	70.616	62.710	26.091	-43.[illegible]64	-74.414	4.928
3400	9.082	70.887	62.946	26.999	-43.5[illegible]	-75.351	4.843
3500	9.092	71.151	63.177	27.908	-43.83[illegible]	-76.283	4.763
3565.77	9.099	71.320	63.326	28.506	-44.024	-76.892	4.713
3565.77	9.099	71.320	63.326	28.506	-135.519	-76.892	4.713
3600	9.102	71.407	63.402	28.818	-135.562	-76.328	4.634
3700	9.112	71.657	63.622	29.728	-135.694	-74.662	4.411
3800	9.123	71.900	63.837	30.640	-135.826	-73.031	4.200
3900	9.135	72.137	64.047	31.553	-135.960	-71.380	4.000
4000	9.147	72.369	64.252	32.467	-136.093	-69.718	3.809
4100	9.160	72.595	64.453	33.382	-136.229	-68.062	3.626
4200	9.174	72.816	64.650	34.299	-136.366	-66.393	3.455
4300	9.189	73.032	64.842	35.217	-136.499	-64.727	3.290
4400	9.205	73.244	65.031	36.137	-136.635	-63.055	3.132
4500	9.223	73.451	65.216	37.058	-136.772	-61.381	2.981
4600	9.242	73.654	65.397	37.982	-136.909	-59.704	2.836
4700	9.262	73.854	65.575	38.907	-137.045	-58.026	2.698
4800	9.284	74.049	65.750	39.834	-137.184	-56.346	2.565
4900	9.307	74.241	65.922	[illegible].764	-137.322	-54.663	2.438
5000	9.333	74.429	66.090	41.695	-137.462	-52.970	2.315
5100	9.360	74.615	66.256	42.630	-137.605	-51.279	2.197
5200	9.389	74.797	66.419	43.568	-137.748	-49.588	2.084
5300	9.421	74.976	66.579	44.508	-137.895	-47.893	1.975
5400	9.454	75.153	66.736	45.452	-138.045	-46.191	1.869
5500	9.489	75.327	66.891	46.399	-138.202	-44.486	1.768
5600	9.527	75.499	67.043	47.350	-138.365	-42.780	1.669
5700	9.567	75.668	67.194	48.304	-138.538	-41.083	1.575
5800	9.608	75.835	67.342	49.265	-138.722	-39.366	1.483
5900	9.652	76.000	67.487	50.226	-138.921	-37.645	1.394
6000	9.699	76.163	67.631	51.193	-139.137	-35.932	1.309

15 June 1963 — HLS

SILICON MONOXIDE (SiO) (IDEAL MOLECULAR GAS) gfw = 44.09

ΔH_{f0} = -24.316 kcal gfw^{-1}
Ground State Configuration $^1\Sigma^+$
$H^\circ_{298.15} - H^\circ_0$ = 2.083 kcal gfw^{-1}

$\Delta H^\circ_{f298.15}$ = -24.04 kcal gfw^{-1}
$S^\circ_{298.15}$ = 50.544 cal deg K^{-1} gfw^{-1}

State	g	E	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e \times 10^5$	$D_e \times 10^6$
		cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}
$^1\Sigma^+$	1	0.0	1241.44	5.92	0.0	0.72729	0.00508	0.0	1.02
$^3\pi_r$	6	32000	1000	6.0	0.0	0.67656	0.0	0.0	1.4

Heat of Formation

As interim measure, the value by Wise *et al*[1] has been used. This value may be modified slightly by using internally self-consistent functions generated on this project.

Heat Capacity and Entropy

Have been calculated using ground-state data by Lagerqvist and Uhler[2] and excited state from Verma and Mulliken.[3]

References

1. Wise, S. S. *et al*, J. Phys. Chem. 67, 815 (1963).
2. Lagerqvist, A. and U. Uhler, Arkiv Physik 6, 95 (1953).
3. Verma, R. D. and R. S. Mulliken, Can. J. Phys. 39, 908 (1961).

SILICON MONOXIDE (SiO) (IDEAL MOLECULAR GAS) GFW = 44.09

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw			Kcal/gfw			
	C°_p	S°_T	$-(F^\circ_T - H^\circ_{298})/T$	$H^\circ_T - H^\circ_{298}$	ΔH_f	ΔF_f	Log K_p
298.15	± 0.005	± 0.005	± 0.005	± 0.000	±0.450		
1000	± 0.005	± 0.006	± 0.005	± 0.005			
2000	± 0.008	± 0.008	± 0.006	± 0.010			
3000	± 0.010	± 0.010	± 0.008	± 0.020			
4000	± 0.040	± 0.012	± 0.009	± 0.030			
5000	± 0.200	± 0.035	± 0.015	± 0.130			
6000	± 0.700	± 0.110	± 0.025	± 0.500			

TABLE 186

STRONTIUM MONOXIDE CONDENSED PHASE **OSr**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Sr from 0° to 1045°K, Liquid Sr from 1045° to 1641°K, Gaseous Sr from 1641° to 4000°K; Gaseous O_2; Solid SrO from 0° to 2690°K, Liquid SrO from 2690° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.038	-140.551	-140.551	INFINITE
298.15	10.760	13.060	13.060	0.000	-141.100	-133.961	98.192
300	10.784	13.127	13.060	0.020	-141.099	-133.917	97.554
400	11.663	16.365	13.496	1.148	-140.987	-131.539	71.866
500	12.138	19.023	14.343	2.340	-140.860	-129.192	56.467
600	12.453	21.265	15.315	3.570	-140.749	-126.868	46.210
700	12.694	23.204	16.307	4.828	-140.661	-124.563	38.888
800	12.894	24.912	17.278	6.108	-140.600	-122.267	33.400
862	13.006	25.879	17.862	6.910	-140.578	-120.847	30.638
862	13.006	25.879	17.862	6.910	-140.778	-120.847	30.638
900	13.071	26.441	18.212	7.406	-140.786	-119.969	29.131
1000	13.233	27.827	19.106	8.721	-140.800	-117.655	25.712
1045	13.303	28.411	19.494	9.318	-140.804	-116.613	24.387
1045	13.303	28.411	19.494	9.318	-142.774	-116.613	24.387
1100	13.386	29.095	19.957	10.052	-142.701	-115.238	22.895
1200	13.532	30.266	20.768	11.398	-142.559	-112.748	20.533
1300	13.674	31.355	21.541	12.758	-142.[illegible]	-110.270	18.537
1400	13.813	32.374	22.279	14.133	-142.245	-107.805	16.828
1500	13.949	33.331	22.984	15.521	-142.072	-105.350	15.349
1600	14.083	34.236	23.659	16.923	-141.888	-102.907	14.056
1640.43	14.138	34.593	23.928	17.501	-141.802	-101.909	13.572
1640.43	14.138	34.593	23.928	17.501	-174.814	-101.909	13.572
1700	14.216	35.094	24.307	18.338	-174.531	-99.288	12.764
1800	14.348	35.910	24.929	19.766	-174.046	-94.877	11.519
1900	14.479	36.689	25.527	21.207	-173.552	-90.492	10.408
2000	14.609	37.435	26.104	22.662	-173.049	-86.133	9.412
2100	14.739	38.151	26.661	24.129	-172.539	-81.801	8.513
2200	14.868	38.840	27.199	25.609	-172.023	-77.490	7.698
2300	14.997	39.503	27.720	27.103	-171.502	-73.204	6.956
2400	15.125	40.144	28.224	28.609	-170.978	-68.943	6.278
2500	15.253	40.764	28.713	30.128	-170.452	-64.705	5.656
2600	15.381	41.365	29.189	31.659	-169.926	-60.482	5.084
2690	15.496	41.891	29.605	33.049	-169.456	-56.707	4.607
2690	17.000	47.876	29.605	49.149	-153.356	-56.707	4.607
2700	17.000	47.939	29.673	49.319	-153.289	-56.344	4.561
2800	17.000	48.557	30.336	51.019	-152.626	-52.766	4.118
2900	17.000	49.154	30.975	52.719	-151.988	-49.211	3.708
3000	17.000	49.730	31.590	54.419	-151.369	-45.675	3.327
3100	17.000	50.287	32.184	56.119	-150.774	-42.160	2.972
3200	17.000	50.827	32.759	57.819	-150.207	-38.669	2.641
3300	17.000	51.350	33.314	59.519	-149.669	-35.190	2.330
3400	17.000	51.858	33.852	61.219	-149.163	-31.731	2.040
3500	17.000	52.350	34.374	62.919	-148.689	-28.282	1.766
3600	17.000	52.829	34.880	64.619	-148.250	-24.850	1.508
3700	17.000	53.295	35.371	66.319	-147.847	-21.428	1.266
3800	17.000	53.749	35.849	68.019	-147.483	-18.012	1.036
3900	17.000	54.190	36.313	69.719	-147.157	-14.611	0.819
4000	17.000	54.621	36.766	71.419	-146.870	-11.217	0.613
4100	17.000	55.040	37.206	73.119	-146.624	-7.827	0.417
4200	17.000	55.450	37.636	74.819	-146.418	-4.444	0.231
4300	17.000	55.850	38.055	76.519	-146.252	-1.061	0.054
4400	17.000	56.241	38.464	78.219	-146.126	2.310	-0.115
4500	17.000	56.623	38.863	79.919	-146.039	5.685	-0.276
4600	17.000	56.996	39.253	81.619	-145.991	9.057	-0.430
4700	17.000	57.362	39.635	83.319	-145.983	12.427	-0.578
4800	17.000	57.720	40.008	85.019	-146.011	15.797	-0.719
4900	17.000	58.070	40.373	86.719	-146.076	19.168	-0.855
5000	17.000	58.414	40.730	88.419	-146.177	22.544	-0.985
5100	17.000	58.751	41.080	90.119	-146.314	25.919	-1.111
5200	17.000	59.081	41.423	91.819	-146.485	29.292	-1.231
5300	17.000	59.405	41.759	93.519	-146.691	32.682	-1.348
5400	17.000	59.722	42.089	95.219	-146.931	36.068	-1.460
5500	17.000	60.034	42.413	96.919	-147.203	39.459	-1.568
5600	17.000	60.341	42.730	98.619	-147.511	42.857	-1.672
5700	17.000	60.641	43.042	100.319	-147.853	46.267	-1.774
5800	17.000	60.937	43.348	102.019	-148.231	49.673	-1.872
5900	17.000	61.228	43.648	103.719	-148.646	53.097	-1.967
6000	17.000	61.513	43.944	105.419	-149.101	56.524	-2.059

15 December 1962 RCF

$\Delta H^o_{f298.15}$ = -141.100 kcal gfw^{-1} $S^o_{298.15}$ = 13.060 cal deg K^{-1}gfw^{-1}

T_m = 2690°K ΔH_m = 16.1 kcal gfw^{-1}

$H^o_{298.15}-H^o_0$ = 2.038 kcal gfw^{-1}

$C^o_p = 12.13 + 1.26 \times 10^{-3}T - 1.55 \times 10^5 T^{-2}$ cal deg K^{-1}gfw^{-1}

$298.15°K \leq T \leq 2690°K$

C^o_p = 17.0 cal deg K^{-1}gfw^{-1} $2690°K \leq T \leq 6000°K$

Structure

An f. c. c. (NaCl) type.

Heat of Formation

Based on data from Rossini *et al.*[1]

Heat Capacity and Entropy

Low-temperature data by Anderson.[2] High-temperature data valid to 1266°K by Lander[3] and Kelley[4] extrapolated to melting point. Liquid heat capacity estimated.

Melting and Vaporization

Heat of fusion estimated. See Barriault *et al*[5] for details.

References

1. Rossini, F. *et al*, Nat. Bur. Stds. (U.S.) Circ. 500 (1952).
2. Anderson, C. T., J. Am. Chem. Soc. 57, 429 (1935).
3. Lander, J. J., J. Am. Chem. Soc. 73, 5794 (1951).
4. Kelley, K. K., U. S. Bur. Mines, Bull. 584 (1960).
5. Barriault, R. J. *et al*, ASD TR 61-260, Pt. I (May 1962).

STRONTIUM MONOXIDE (SrO) (CONDENSED PHASE) GFW = 103.63

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw C^o_p	S^o_T	$-(F^o_T - H^o_{298})/T$	kcal gfw $H^o_T - H^o_{298}$	ΔH^o_f	ΔF_f	Log K_p
298.15	± 0.200	± 0.200	± 0.200	± 0.000	± 2.000	± 2.210	± 1.620
1000	± 0.940	± 0.650	± 0.390	± 0.260	± 2.440	± 2.960	± 0.650
2000	± 1.780	± 0.940	± 0.600	± 0.680	± 3.730	± 4.250	± 0.460
2690	± 2.680	± 1.070	± 0.700	± 0.990	± 4.040	± 4.930	± 0.400
2690	± 1.000	± 1.590	± 0.700	± 2.390	± 5.440	± 4.930	± 0.400
4000	± 2.000	± 2.190	± 1.100	± 4.350	± 7.400	± 7.450	± 0.410

TABLE 187

STRONTIUM MONOXIDE IDEAL MOLECULAR GAS **OSr**

Reference State for Calculating ΔH°_f, ΔF°_f and Log K_p: Solid Sr from 0° to 1045°K, Liquid Sr from 1045° to 1641°K, Gaseous Sr from 1641° to 6000°K; Gaseous O_2; Gaseous SrO.

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal/gfw)	ΔH°_f (Kcal/gfw)	ΔF°_f (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.161	-11.874	-11.874	INFINITE
298.15	7.910	57.145	57.145	0.000	-12.300	-18.305	13.417
300	7.918	57.194	57.145	0.015	-12.303	-18.342	13.362
400	8.277	59.525	57.460	0.826	-12.509	-20.325	11.104
500	8.501	61.398	58.067	1.666	-12.734	-22.254	9.727
600	8.644	62.961	58.756	2.523	-12.996	-24.133	8.790
700	8.742	64.302	59.454	3.393	-13.295	-25.966	8.107
800	8.813	65.474	60.135	4.271	-13.637	-27.753	7.581
862	8.848	66.133	60.543	4.818	-13.870	-28.838	7.311
862	8.848	66.133	60.543	4.818	-14.070	-28.838	7.311
900	8.866	65.515	60.787	5.155	-14.236	-29.486	7.160
1000	8.909	67.452	61.408	6.044	-14.677	-31.157	6.809
1045	8.925	67.844	61.676	6.445	-14.878	-31.894	6.670
1045	8.925	67.844	61.676	6.445	-16.848	-31.894	6.670
1100	8.944	68.302	61.996	6.936	-17.017	-32.681	6.493
1200	8.973	69.082	62.555	7.832	-17.325	-34.093	6.209
1300	9.000	69.801	63.085	8.731	-17.634	-35.477	5.964
1400	9.024	70.469	63.589	9.632	-17.946	-36.839	5.751
1500	9.046	71.093	64.069	10.536	-18.257	-38.177	5.562
1600	9.068	71.677	64.526	11.442	-18.569	-39.494	5.394
1640.43	9.077	71.907	64.708	11.813	-18.690	-40.029	5.331
1640.43	9.077	71.907	64.708	11.813	-51.702	-40.029	5.331
1700	9.089	72.228	64.963	12.349	-51.720	-39.604	5.091
1800	9.111	72.748	65.387	13.259	-51.753	-38.892	4.722
1900	9.132	73.242	65.783	14.172	-51.787	-38.177	4.391
2000	9.155	73.711	66.168	15.086	-51.825	-37.460	4.093
2100	9.177	74.156	66.538	16.002	-51.866	-36.743	3.824
2200	9.201	74.586	66.895	16.921	-51.912	-36.022	3.578
2300	9.226	74.996	67.238	17.843	-51.962	-35.297	3.354
2400	9.252	75.390	67.570	18.767	-52.020	-34.573	3.148
2500	9.276	75.768	67.891	19.693	-52.087	-33.849	2.959
2600	9.305	76.133	68.201	20.622	-52.164	-33.116	2.784
2690	9.331	76.451	68.473	21.461	-52.245	-32.460	2.637
2690	9.331	76.451	68.473	21.461	-52.245	-32.460	2.637
2700	9.334	76.485	68.502	21.554	-52.254	-32.384	2.621
2800	9.363	76.826	68.794	22.489	-52.358	-31.648	2.470
2900	9.392	77.156	69.077	[illegible]	-52.460	-30.908	2.329
3000	9.423	77.475	69.353	24.367	-52.621	-30.163	2.197
3100	9.454	77.785	69.620	[illegible]	-52.782	-29.410	2.073
3200	9.486	78.087	69.881	26.258	-52.968	-28.660	1.957
3300	9.518	78.380	70.135	27.208	[illegible]	-27.899	1.848
3400	9.551	78.666	70.383	28.167	-53.420	-27.136	1.744
3500	9.585	78.944	70.674	29.119	-53.689	-26.358	1.646
3600	9.619	79.216	70.860	30.079	-53.990	-25.579	1.553
3700	9.653	79.481	71.091	31.042	-54.324	-24.791	1.464
3800	9.688	79.740	71.316	32.009	-54.692	-23.987	1.379
3900	9.724	79.993	71.537	32.980	-55.096	-23.183	1.299
4000	9.760	80.241	71.753	33.954	-55.535	-22.366	1.222
4100	9.796	80.484	71.964	34.931	-56.012	-21.533	1.148
4200	9.833	80.722	72.171	35.912	-56.525	-20.692	1.077
4300	9.870	80.955	72.375	36.897	-57.074	-19.838	1.008
4400	9.908	81.184	72.574	37.886	-57.659	-18.975	0.942
4500	9.946	81.409	72.769	38.878	-58.280	-18.092	0.879
4600	9.985	81.630	72.962	39.875	-58.935	-17.204	0.817
4700	10.024	81.847	73.150	40.875	-59.627	-16.295	0.758
4800	10.063	82.060	73.336	41.879	-60.351	-15.379	0.700
4900	10.103	82.270	73.518	42.887	-61.108	-14.444	0.644
5000	10.144	82.477	73.697	43.899	-61.897	-13.490	0.590
5100	10.184	82.681	73.874	44.915	-62.718	-12.530	0.537
5200	10.226	82.881	74.048	45.935	-63.569	-11.556	0.486
5300	10.267	83.079	74.219	46.959	-64.450	-10.554	0.435
5400	10.310	83.274	74.387	47.987	-65.363	-9.541	0.386
5500	10.352	83.466	74.553	49.020	-66.302	-8.513	0.338
5600	10.395	83.656	74.717	50.056	-67.274	-7.470	0.292
5700	10.439	83.843	74.878	51.097	-68.275	-6.400	0.245
5800	10.482	84.028	75.038	52.143	-69.307	-5.331	0.201
5900	10.526	84.210	75.195	53.193	-70.372	-4.229	0.157
6000	10.571	84.391	75.350	54.247	-71.473	-3.114	0.113

15 December 1962 RCF

STRONTIUM MONOXIDE (SrO) (IDEAL MOLECULAR GAS) gfw = 103.63

ΔH^o_{f0} = -11.874 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = -12.300 kcal gfw^{-1}

Ground State Configuration = $^3\Sigma$

$S^o_{298.15}$ = 57.145 cal deg K^{-1}gfw^{-1}

$H^o_{298.15}-H^o_0$ = 2.161 kcal gfw^{-1}

State	g	E	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e \times 10^5$	$D_e \times 10^6$
		cm^{-1}							
$X\ ^3\Sigma$	3	0	653.47	3.95	—	0.3379	0.0021	—	0.42
$A'\ ^1\Sigma$	1	10885	619.6	0.9	—	0.3047	0.0011	—	3.2
$B'\ ^1\Sigma$	2	24004.0	520.0	3.5	—	0.2936	0.002	—	0.37
$C'\ ^1\Sigma$	1	28546.4	480.2	2.6	—	0.2742	0.0021	—	0.35

Heat of Formation

Calculated from vapor-pressure data analyzed by Ackermann and Thorn,[1] based on work of Moore *et al.*[2]

Heat Capacity and Entropy

Calculated using above spectroscopic constants. See volume 1, this study (section IVB26.4) and Barriault *et al*[3] for details.

References

1. Ackermann, R. and R. Thorn, p. 50 of *Prog. Ceramics Science*, edited by J. E. Burke, Pergamon Press (1961).
2. Moore, G. E. *et al*, J. Chem. Phys. 18, 1572 (1950).
3. Barriault, R. *et al*, ASD TR 61-260, Pt. I (May 1962).

TABLE 188

TANTALUM MONOXIDE IDEAL MOLECULAR GAS **OTa**

Reference State for Calculating ΔH_f^o, ΔF_f^o, and Log K_p: Solid Ta from 0° to 3270°K, Liquid Ta from 3270° to 5706°K, Gaseous Ta from 5706° to 6000°K; Gaseous O_2; Gaseous TaO.

T, °K	C_p^o (cal/°K gfw)	S_T^o (cal/°K gfw)	$-(F_T^o - H_{298}^o)/T$ (cal/°K gfw)	$H_T^o - H_{298}^o$ (Kcal/gfw)	ΔH_f^o (Kcal/gfw)	ΔF_f^o (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.258	52.110	52.110	INFINITE
298.15	7.954	58.568	58.568	0.000	51.973	44.774	-32.819
300	7.956	58.618	58.568	0.015	51.970	44.730	-32.584
400	8.116	60.927	58.882	0.818	51.799	42.341	-23.133
500	8.287	62.757	59.480	1.638	51.621	39.997	-17.482
600	8.431	64.281	60.157	2.474	51.437	37.690	-13.728
700	8.542	65.589	60.842	3.323	51.248	35.413	-11.056
800	8.628	66.736	61.508	4.182	51.052	33.165	- .060
900	8.694	67.756	62.147	5.048	50.851	30.940	-7.513
1000	8.745	68.674	62.754	5.920	50.643	28.739	-6.281
1100	8.787	69.510	63.331	6.797	50.432	26.559	-5.277
1200	8.820	70.276	63.878	7.677	50.213	24.399	-4.443
1300	8.848	70.983	64.398	8.561	49.989	22.256	-3.741
1400	8.872	71.640	64.892	9.447	49.758	20.131	-3.143
1500	8.892	72.253	65.363	10.335	49.518	18.023	-2.626
1600	8.910	72.827	65.811	11.225	49.271	15.932	-2.176
1700	8.925	73.368	66.240	12.117	49.015	13.856	-1.781
1800	8.939	73.878	66.650	13.010	48.749	11.796	-1.432
1900	8.952	74.362	67.044	13.905	48.474	9.748	-1.121
2000	8.964	74.822	67.421	14.801	48.185	7.719	-0.843
2100	8.974	75.259	67.784	15.697	47.882	5.703	-0.593
2200	8.984	75.677	68.134	16.595	47.566	3.702	-0.368
2300	8.994	76.077	68.470	17.494	47.233	1.717	-0.163
2400	9.003	76.460	68.795	18.394	46.882	-0.257	0.023
2500	9.012	76.827	69.109	19.295	46.505	-2.213	0.193
2600	9.020	77.181	69.413	20.197	46.108	-4.154	0.349
2700	9.029	77.522	69.707	21.099	45.674	-6.078	0.492
2800	9.037	77.850	69.992	22.002	45.199	-7.989	0.624
2900	9.045	78.168	70.269	22.906	44.671	-9.880	0.745
3000	9.054	78.474	70.537	23.811	44.080	-11.751	0.856
3100	9.063	78.772	70.798	24.717	43.419	-13.600	0.959
3200	9.072	79.060	71.052	25.624	42.679	-15.430	1.054
3270	9.079	79.256	71.226	26.259	42.111	-16.695	1.116
3270	9.079	79.256	71.226	26.259	35.411	-16.695	1.116
3300	9.081	79.339	71.299	26.532	35.284	-17.172	1.137
3400	9.091	79.610	71.540	[illegible].440	34.857	-18.759	1.206
3500	9.102	79.874	71.774	28.350	34.430	-20.325	1.269
3600	9.113	80.131	72.003	29.261	34.002	-21.886	1.329
3700	9.125	80.381	72.226	30.173	33.574	-23.433	1.384
3800	9.138	80.625	72.444	31.086	33.144	-24.967	1.436
3900	9.152	80.862	72.657	32.000	32.714	-26.493	1.485
4000	9.166	81.094	72.865	32.916	32.284	-28.005	1.530
4100	9.182	81.321	73.069	33.834	31.854	-29.510	1.573
4200	9.199	81.543	73.268	34.753	31.423	-30.998	1.613
4300	9.216	81.760	73.464	35.673	30.991	-32.483	1.651
4400	9.235	81.972	73.655	36.596	30.560	-33.955	1.686
4500	9.255	82.180	73.842	37.520	30.129	-35.417	1.720
4600	9.276	82.384	74.026	38.447	29.698	-36.867	1.751
4700	9.298	82.584	74.206	39.376	29.266	-38.309	1.781
4800	9.321	82.780	74.383	40.307	28.834	-39.743	1.809
4900	9.346	82.973	74.557	41.240	28.400	-41.174	1.836
5000	9.371	83.162	74.727	42.176	27.966	-42.587	1.861
5100	9.397	83.348	74.895	43.114	27.529	-43.994	1.885
5200	9.425	83.532	75.059	44.055	27.090	-45.392	1.908
5300	9.454	83.712	75.221	44.999	26.647	-46.785	1.929
5400	9.483	83.889	75.381	45.946	26.200	-48.170	1.949
5500	9.514	84.064	75.537	46.896	25.748	-49.538	1.968
5600	9.545	84.236	75.692	47.849	25.287	-50.907	1.987
5700	9.577	84.406	75.843	48.805	24.817	-52.263	2.004
5706.65	9.580	84.417	75.853	48.869	24.786	-52.353	2.005
5706.65	9.580	84.417	75.853	48.869	-156.436	-52.353	2.005
5800	9.611	84.573	75.993	49.764	-157.041	-50.649	1.908
5900	9.644	84.738	76.140	50.727	-157.707	-48.811	1.808
6000	9.679	84.901	76.285	51.693	-158.394	-46.955	1.710

15 September 1963 HLS

TANTALUM MONOXIDE (TaO) (IDEAL MOLECULAR GAS) gfw = 196.95

ΔH°_{f0} = 52.110 kcal gfw^{-1}

$\Delta H^\circ_{f298.15}$ = 51.973 kcal gfw^{-1}

Ground State Configuration $^2\Delta$

$S^\circ_{298.15}$ = 58.568 cal deg^{-1} gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 2.258 kcal gfw^{-1}

			cm^{-1}						
State	g	E	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e \times 10^5$	$D_e \times 10^6$
a $^2\Delta_{3/2}$	2	0	1013.17	5.0	0.0	0.4029	0.002	0.0	0.0
a $^2\Delta_{5/2}$	2	300.							
b $^2\pi_{1/2}$	2	23348	896.	4.1	0.0	0.3772	0.0019	0.0	0.0
b $^2\pi_{3/2}$	2	24364	898.5						
c $^2\Delta$	4	26679	903.01	4.15	0.0	0.3775	0.0019	0.0	0.0

Heat of Formation

Vaporization data reported by Inghram *et al*[1] were analyzed.

Heat Capacity and Entropy

Calculated using spectroscopic constants above, based primarily on the work of Premaswarup and Barrow.[2]

References

1. Inghram, M. G., *et al*, J. Chem. Phys. 27, 569 (1957).
2. Premaswarup, D. and R. F. Barrow, Nature 180, 602 (1957).

TANTALUM MONOXIDE (TaO) (IDEAL MOLECULAR GAS) GFW = 196.95

SUMMARY OF UNCERTAINTY ESTIMATES

T °K	C_p (cal/°K gfw)	S_T	$-(F_T - H_{298})/T$	$H_T - H_{298}$ (kcal/gfw)	ΔH_f	ΔF_f	Log K_p
298.15	±1.000	±1.000	±1.000	±0.000	±5.000		
1000	±1.000	±2.210	±1.508	±0.702			
2000	±1.000	±2.903	±2.052	±1.702			
3000	±1.000	±3.309	±2.408	±2.702			
4000	±1.000	±3.596	±2.671	±3.702			
5000	±1.000	±3.820	±2.879	±4.702			
6000	±1.000	±4.002	±3.052	±5.702			

TABLE 189

TECHNETIUM MONOXIDE IDEAL MOLECULAR GAS

OTc

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p. Solic Tc from 0° to 2473°K, Liquid Tc from 2473° to 4840°K, Gaseous Tc from 4840° to 6000°K; Gaseous O_2; Gaseous TcO.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.114	89.004	89.004	INFINITE
298.15	7.521	57.538	57.538	0.000	88.600	81.136	-59.471
300	7.529	57.584	57.538	0.014	88.597	81.090	-59.071
400	7.911	59.805	57.838	0.787	88.425	78.614	-42.950
500	8.185	61.602	58.417	1.592	88.253	76.181	-33.297
600	8.373	63.112	59.077	2.421	88.074	73.783	-26.874
700	8.502	64.413	59.748	3.265	87.880	71.416	-22.296
800	8.594	65.554	60.404	4.120	87.664	69.079	-18.871
900	8.661	66.571	61.034	4.983	87.431	66.769	-16.213
1000	8.710	67.486	61.634	5.852	87.175	64.488	-14.093
1100	8.748	68.318	62.204	6.725	86.898	62.232	-12.364
1200	8.778	69.080	62.746	7.601	86.600	60.002	-10.927
1300	8.801	69.784	63.261	8.480	86.280	57.798	-9.716
1400	8.820	70.437	63.750	9.361	85.939	55.620	-8.682
1500	8.835	71.046	64.217	10.244	85.576	53.466	-7.790
1600	8.848	71.617	64.662	11.128	85.191	51.338	-7.012
1700	8.858	72.153	65.087	12.013	84.784	49.235	-6.329
1800	8.867	72.660	65.493	12.900	84.356	47.158	-5.725
1900	8.875	73.140	65.883	13.787	83.9[illegible]	45.102	-5.188
2000	8.881	73.595	66.258	14.675	83.433	43.072	-4.706
2100	8.887	74.028	66.617	15.563	82.938	41.068	-4.274
2200	8.892	74.442	66.964	16.452	82.422	39.084	-3.882
2300	8.896	74.837	67.298	17.341	81.881	37.125	-3.527
2400	8.900	75.216	67.620	18.231	81.320	35.192	-3.204
2473	8.902	75.483	67.848	18.881	80.896	33.796	-2.987
2473	8.902	75.483	67.848	18.881	75.208	33.796	-2.987
2500	8.903	75.579	67.931	19.121	75.053	33.344	-2.915
2600	8.906	75.929	68.232	20.012	74.478	31.687	-2.663
2700	8.909	76.265	68.523	20.903	73.900	30.052	-2.432
2800	8.911	76.565	68.805	21.794	73.320	28.439	-2.220
2900	8.913	76.902	69.079	22.685	72.737	26.846	-2.023
3000	8.915	77.204	69.345	23.576	72.152	25.275	-1.841
3100	8.917	77.496	69.603	24.468	71.565	2[illegible].722	-1.672
3200	8.918	77.779	69.854	25.360	70.976	22.189	-1.515
3300	8.920	78.054	70.099	26.251	70.385	20.670	-1.369
3400	8.921	78.320	70.337	27.144	69.793	19.174	-1.232
3500	8.922	78.579	70.568	28.036	69.198	17.699	-1.105
3600	8.923	78.830	70.794	28.928	68.601	16.235	-0.986
3700	8.925	79.074	71.015	29.820	68.002	4.785	-0.873
3800	8.925	79.312	71.230	30.713	67.403	13.358	-0.768
3900	8.926	79.544	71.440	31.605	66.800	11.944	-0.669
4000	8.927	79.770	71.646	32.498	66.19[illegible]	10.542	-0.576
4100	8.928	79.9[illegible]	71.847	33.391	65.592	9.158	-0.488
4200	8.929	80.206	72.043	34.284	64.985	7.792	-0.405
4300	8.929	80.416	72.235	35.177	64.377	6.440	-0.327
4400	8.930	80.621	72.424	36.070	63.766	5.097	-0.253
4500	8.930	80.822	72.608	36.963	63.153	3.770	-0.183
4600	8.931	81.018	72.789	37.856	62.538	2.456	-0.117
4700	8.931	81.210	72.966	38.749	61.921	1.161	-0.054
4800	8.932	81.398	73.140	39.642	61.300	-0.126	0.006
4840.07	8.932	81.472	73.208	39.999	61.050	-0.640	0.029
4840.07	8.932	81.472	73.208	39.999	-78.[illegible]	-0.640	0.029
4900	8.932	81.583	73.310	40.535	-79.045	0.[illegible]	-0.015
5000	8.933	81.763	73.477	41.428	-79.426	1.9[illegible]	-0.086
5100	8.933	81.940	73.642	42.[illegible]	-79.815	3.588	-0.154
5200	8.933	82.113	73.8[illegible]3	43.21[illegible]	-80.213	5.234	-0.220
5300	8.934	82.284	73.961	44.108	-80.621	6.877	-0.284
5400	8.934	82.451	74.11[illegible]	45.002	-81.039	8.534	-0.345
5500	8.934	82.614	74.270	45.895	-81.469	10.200	-0.405
5600	8.935	82.775	74.420	46.789	-81.912	11.877	-0.464
5700	8.935	82.934	74.568	47.682	-82.371	13.554	-0.520
5800	8.935	83.069	74.714	48.576	-82.848	15.239	-0.574
5900	8.936	83.242	74.8[illegible]	49.469	-83.346	16.939	-0.627
6000	8.936	83.39[illegible]	74.998	50.363	-83.868	18.646	-0.679

15 December 1962 RCF

TECHNETIUM MONOXIDE (TcO) (IDEAL MOLECULAR GAS) gfw = 115

ΔH^o_{f0} = 89.004 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 88.600 kcal gfw^{-1}

Ground State Degeneracy = 4

$S^o_{298.15}$ = 57.538 cal deg K^{-1}gfw^{-1}

$H^o_{298.15} - H^o_0$ = 2.114 kcal gfw^{-1}

State	g	E	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e \times 10^5$	$D_e \times 10^6$
		cm^{-1}							
X	4	0	854	---	---	0.385	---	---	---

Heat of Formation

Estimated by comparison of dissociation energies of oxides of neighboring elements in periodic table .

Heat Capacity and Entropy

Calculated using above estimated spectroscopic constants.

TABLE 190

THORIUM MONOXIDE — IDEAL MOLECULAR GAS — **ThO**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p. Solid Th from 0° to 2028°K, Liquid Th from 2028° to 5060°K, Gaseous Th from 5060° to 6000°K, Gaseous O_2; Gaseous ThO.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.125	-7.172	-7.172	INFINITE
298.15	7.627	58.836	58.836	0.000	-7.640	-14.399	10.554
300	7.636	58.883	58.836	0.014	-7.649	-14.441	10.520
400	8.033	61.137	59.141	0.798	-8.084	-16.639	9.091
500	8.340	62.963	59.728	1.618	-8.493	-18.730	8.186
600	8.602	64.508	60.399	2.465	-8.888	-20.739	7.554
700	8.851	65.852	61.084	3.338	-9.268	-22.684	7.082
800	9.095	67.050	61.756	4.235	-9.634	-24.576	6.713
900	9.331	68.135	62.406	5.156	-9.984	-26.423	6.416
1000	9.551	69.130	63.029	6.101	-10.317	-28.231	6.169
1100	9.750	70.050	63.626	7.066	-10.635	-30.007	5.962
1200	9.923	70.906	64.198	8.050	-10.939	-31.755	5.783
1300	10.067	71.706	64.745	9.050	-11.232	-33.478	5.628
1400	10.183	72.456	65.269	10.062	-11.516	-35.178	5.491
1500	10.273	73.162	65.772	11.085	-11.792	-36.859	5.370
1600	10.338	73.827	66.255	12.116	-12.063	-38.521	5.261
1633	10.354	74.039	66.410	12.457	-12.152	-39.066	5.228
1633	10.354	74.039	66.410	12.457	-12.806	-39.066	5.228
1700	10.382	74.456	66.719	13.152	-13.144	-40.137	5.160
1800	10.408	75.050	67.166	14.192	-13.648	-41.711	5.064
1900	10.419	75.613	67.595	15.233	-14.154	-43.255	4.975
2000	10.418	76.147	68.010	16.275	-14.662	-44.774	4.892
2028	10.417	76.292	68.123	16.567	-14.805	-45.195	4.870
2028	10.417	76.292	68.123	16.567	-18.658	-45.195	4.870
2100	10.408	76.656	68.410	17.317	-19.026	-46.130	4.801
2200	10.391	77.140	68.796	18.357	-19.542	-47.408	4.709
2300	10.368	77.601	69.169	19.395	-20.062	-48.664	4.624
2400	10.342	78.042	69.529	20.430	-20.588	-49.896	4.543
2500	10.312	78.464	69.879	21.463	-21.119	-51.109	4.468
2600	10.281	78.868	70.217	22.493	-21.655	-52.296	4.396
2700	10.249	79.255	70.544	23.519	-22.197	-53.466	4.328
2800	10.217	79.628	70.862	24.542	-22.745	-54.613	4.263
2900	10.186	79.986	71.171	25.563	-23.299	-55.744	4.201
3000	10.154	80.331	71.471	26.580	-23.858	-56.854	4.142
3100	10.124	80.664	71.762	27.594	-24.422	-57.942	4.085
3200	10.095	80.985	72.046	28.604	-24.973	-59.018	4.031
3300	10.067	81.295	72.322	29.613	-25.56[illegible]	-60.074	3.978
3400	10.040	81.596	72.590	30.618	-26.14[illegible]	-61.107	3.928
3500	10.015	81.887	72.852	31.621	-26.7[illegible]	-62.130	3.879
3600	9.991	82.169	73.107	32.621	-27.320	-63.132	3.832
3700	9.969	82.443	73.356	33.619	-27.912	-64.121	3.787
3800	9.948	82.709	73.599	34.615	-28.509	-65.094	3.744
3900	9.928	82.967	73.837	35.609	-29.109	-66.052	3.701
4000	9.910	83.219	74.069	36.600	-29.714	-66.994	3.660
4100	9.893	83.464	74.295	37.591	-30.321	-67.918	3.620
4200	9.877	83.702	74.517	38.579	-30.933	-68.830	3.581
4300	9.862	83.935	74.734	39.566	-31.548	-69.728	3.544
4400	9.849	84.162	74.956	40.552	-32.166	-70.652	3.509
4500	9.836	84.384	75.154	41.536	-32.787	-71.477	3.471
4600	9.825	84.601	75.357	42.519	-33.412	-72.330	3.436
4700	9.815	84.813	75.557	43.501	-34.041	-73.177	3.403
4800	9.805	85.020	75.753	44.482	-34.673	-74.002	3.369
4900	9.797	85.223	75.945	45.462	-35.309	-74.817	3.337
5000	9.790	85.421	76.133	46.441	-35.951	-75.620	3.305
5060.26	9.785	85.538	76.244	47.029	-36.341	-76.092	3.286
5060.26	9.785	85.538	76.244	47.029	-159.106	-76.092	3.286
5100	9.783	85.616	76.318	47.420	-159.296	-75.450	3.233
5200	9.777	85.806	76.499	48.398	-159.785	-73.805	3.102
5300	9.772	85.993	76.677	49.375	-160.286	-72.144	2.975
5400	9.767	86.177	76.852	50.352	-160.798	-70.480	2.652
5500	9.763	86.357	77.025	51.329	-161.321	-68.814	2.734
5600	9.760	86.534	77.194	52.305	-161.860	-67.126	2.620
5700	9.758	86.708	77.360	53.281	-162.414	-65.432	2.509
5800	9.756	86.878	77.524	54.257	-162.986	-63.729	2.401
5900	9.755	87.046	77.685	55.232	-163.580	-62.014	2.297
6000	9.754	87.211	77.843	56.207	-164.198	-60.290	2.196

15 December 1962 — RCF

ΔH^o_{f0} = -7.172 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = -7.640 kcal gfw^{-1}

Ground State Configuration = $^3\pi_0$

$S^o_{298.15}$ = 58.836 cal deg K^{-1}gfw^{-1}

$H^o_{298.15}-H^o_0$ = 2.125 kcal gfw^{-1}

State	g	E (cm^{-1})	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	γ_ex10^5	D_ex10^6
$X^3\pi$	2	0							
	2	2721	800	3.5	—	0.327	0.0018	—	0.22
	2	4177							

Heat of Formation

Calculated from data of Darnell et al.[1]

Heat Capacity and Entropy

Calculated using spectroscopic constants above,which are based on Krishnamurty experimental data[2] and data estimated here.

References

1. Darnell, A. J. et al, J. Phys. Chem. 64, 341 (1960).
2. Krishnamurty, S. G., Proc. Phys. Soc. (London) 64A, 852 (1951).

TITANIUM MONOXIDE

CONDENSED PHASE

OTi

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ti from 0° to 1950°K, Liquid Ti from 1950° to 3550°K, Gaseous Ti from 3550° to 6000°K; Gaseous O_2; Solid TiO from 0° to 2010°K, Liquid TiO from 2010° to 6000°K.

T, °K	cal/°K gfw C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	Kcal/gfw $H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.473	-123.436	-123.436	INFINITE
298.15	9.551	9.990	9.990	0.000	-124.150	-117.637	86.226
300	9.583	10.049	9.990	0.018	-124.149	-117.597	85.665
400	10.847	12.998	10.384	1.046	-124.096	-115.419	63.059
500	11.626	15.507	11.164	2.177	-123.985	-113.261	49.504
600	12.213	17.681	12.073	3.365	-123.843	-111.129	40.477
700	12.710	19.602	13.014	4.611	-123.679	-109.023	34.037
800	13.159	21.329	13.947	5.905	-123.494	-106.942	29.214
900	13.580	22.903	14.856	7.242	-123.289	-104.884	25.468
1000	13.984	24.355	15.734	8.621	-123.064	-102.850	22.477
1100	14.376	25.706	16.580	10.039	-122.820	-100.842	20.034
1155	14.589	26.413	17.031	10.835	-122.676	-99.745	18.873
1155	14.589	26.413	17.031	10.835	-123.626	-99.745	18.873
1200	14.761	26.974	17.394	11.496	-123.503	-98.817	17.996
1264	15.004	27.747	17.899	12.448	-123.320	-97.506	16.858
1264	15.642	28.396	17.899	13.268	-122.500	-97.506	16.858
1300	15.750	28.836	18.195	13.833	-122.372	-96.796	16.272
1400	16.050	30.014	18.998	15.423	-122.004	-94.842	14.805
1500	16.350	31.132	19.770	17.043	-121.619	-92.916	13.537
1600	16.650	32.197	20.514	18.693	-121.219	-91.016	12.432
1700	16.950	33.215	21.231	20.373	-120.801	-89.140	11.459
1800	17.250	34.193	21.924	22.083	-120.367	-87.290	10.598
1900	17.550	35.133	22.595	23.823	-119.915	-85.465	9.830
1950	17.700	35.591	22.922	24.704	-119.682	-84.560	9.477
1950	17.700	35.591	22.922	24.704	-123.382	-84.560	9.477
2000	17.850	36.041	23.244	25.593	-123.120	-83.568	9.131
2010	17.880	36.130	23.308	25.772	-123.066	-83.370	9.065
2010	14.500	43.095	23.308	39.772	-109.066	-83.370	9.065
2100	14.500	43.731	24.170	41.077	-108.889	-82.225	8.557
2200	14.500	44.405	25.075	42.527	-108.694	-80.961	8.042
2300	14.500	45.050	25.929	43.977	-108.502	-79.704	7.573
2400	14.500	45.667	26.739	45.427	-108.313	-78.455	7.144
2500	14.500	46.259	27.508	46.877	-108.127	-77.216	6.750
2600	14.500	46.827	28.240	48.327	-107.943	-75.981	6.386
2700	14.500	47.375	28.939	49.777	-107.762	-74.758	6.051
2800	14.500	47.902	29.607	51.227	-107.583	-73.537	5.740
2900	14.500	48.411	30.246	52.677	-107.407	-72.323	5.450
3000	14.500	48.902	30.860	54.127	-107.233	-71.117	5.181
3100	14.500	49.378	31.450	55.577	-107.067	-69.917	4.929
3200	14.500	49.838	32.017	57.027	-106.893	-68.721	4.693
3300	14.500	50.284	32.564	58.477	-106.725	-67.529	4.472
3400	14.500	50.717	33.092	59.927	-106.560	-66.345	4.264
3500	14.500	51.137	33.601	61.377	-106.397	-65.163	4.069
3550	14.500	51.343	33.850	62.102	-106.316	-64.577	3.975
3550	14.500	51.343	33.850	62.102	-208.773	-64.577	3.975
3600	14.500	51.546	34.094	62.827	-208.698	-62.545	3.797
3700	14.500	51.943	34.571	64.277	-208.559	-58.486	3.454
3800	14.500	52.330	35.033	65.727	-208.435	-54.430	3.130
3900	14.500	52.707	35.482	67.177	-208.329	-50.383	2.823
4000	14.500	53.074	35.917	68.627	-208.234	-46.332	2.531
4100	14.500	53.432	36.340	70.077	-208.155	-42.285	2.254
4200	14.500	53.781	36.751	71.527	-208.090	-38.239	1.990
4300	14.500	54.122	37.151	72.977	-208.038	-34.194	1.738
4400	14.500	54.456	37.540	74.427	-208.000	-30.148	1.497
4500	14.500	54.782	37.920	75.877	-207.975	-26.113	1.268
4600	14.500	55.100	38.290	77.327	-207.962	-22.067	1.048
4700	14.500	55.412	38.651	78.777	-207.962	-18.029	0.838
4800	14.500	55.717	39.003	80.227	-207.975	-13.983	0.637
4900	14.500	56.016	39.348	81.677	-207.999	-9.943	0.443
5000	14.500	56.309	39.684	83.127	-208.036	-5.900	0.258
5100	14.500	56.596	40.013	84.577	-208.086	-1.857	0.080
5200	14.500	56.878	40.334	86.027	-208.148	2.189	-0.092
5300	14.500	57.154	40.649	87.477	-208.223	6.238	-0.257
5400	14.500	57.425	40.957	88.927	-208.313	10.283	-0.416
5500	14.500	57.691	41.259	90.377	-208.418	14.337	-0.570
5600	14.500	57.953	41.555	91.827	-208.539	18.384	-0.717
5700	14.500	58.209	41.845	93.277	-208.678	22.443	-0.860
5800	14.500	58.461	42.129	94.727	-208.838	26.502	-0.999
5900	14.500	58.709	42.408	96.177	-209.021	30.566	-1.132
6000	14.500	58.953	42.682	97.627	-209.229	34.628	-1.261

31 December 1963 HLS

TITANIUM MONOXIDE (TiO) (CONDENSED PHASE) gfw = 63.90

$\Delta H^o_{f298.15} = -124.15$ kcal gfw^{-1}

$S^o_{298.15} = 9.99$ cal degK^{-1}gfw^{-1}

$T_t = 1264^oK$

$\Delta H_t = 0.820$ kcal gfw^{-1}

$T_m = 2010^oK$

$\Delta H_m = 14.0$ kcal gfw^{-1}

$H^o_{298.15} - H^o_0 = 1.473$ kcal gfw^{-1}

$C^o_p = 10.57 + 3.60 \times 10^{-3}T - 1.86 \times 10^5 T^{-2}$ cal degK^{-1}gfw^{-1} $\quad 298.15^oK \leq T \leq 1264^oK$

$C^o_p = 11.85 + 3.0 \times 10^{-3}T$ cal degK^{-1}gfw^{-1} $\quad 1264^oK \leq T \leq 2010^oK$

$C^o_p = 14.5$ cal degK^{-1}gfw^{-1} $\quad 2010^oK \leq T \leq 6000^oK$

Structure

TiO has an f. c. c. NaCl (B1) type structure with random vacancies of titanium and oxygen lattices.

Heat of Formation

Based on combustion calorimetry of Mah *et al.*[1]

Heat Capacity and Entropy

Low-temperature data measured by Shomate.[2] An additional entropy contribution of 1.68 e.u. added to account for random vacant Ti and O vacancies as noted by Hoch *et al.*[3] High-temperature data of Naylor[4] valid to 1800°K extrapolated to melting point. Other data estimated.

Melting and Vaporization

Melting point from Brewer.[5] Heat of fusion estimated by Kubaschewski and Evans.[6]

References

1. Mah, A. D. *et al*, U.S. Bur. of Mines, Rept. 5316 (1957).
2. Shomate, C., J. Am. Chem. Soc. 68, 310 (1946).
3. Hoch, M. *et al*, J. Phys. Chem. Solids 23, 1463 (1962).
4. Naylor, B. F., J. Am. Chem. Soc. 68, 1077 (1946).
5. Brewer, L., Chem. Revs. 52, 1-75 (1953).
6. Kubaschewski, O. and E. Evans, *Metallurgical Thermochemistry*, Pergamon Press, New York (1958).

TITANIUM MONOXIDE (TiO) (CONDENSED PHASE) GFW = 63.90

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T (cal/°K gfw)	$-(F^o_T - H^o_{298})/T$ (cal/°K gfw)	$H^o_T - H^o_{298}$ (Kcal/gfw)	ΔH^o_f (Kcal/gfw)	ΔF^o_f (Kcal/gfw)	Log K_p
298.15	± 0.300	± 0.500	± 0.500	± 0.000	± 1.000		
1000	± 0.300	± 0.863	± 0.652	± 0.211			
1264	± 0.300	± 0.933	± 0.704	± 0.290			
1264	± 1.000	± 1.012	± 0.704	± 0.390			
2000	± 1.000	± 1.471	± 0.908	± 1.126			
2010	± 1.000	± 1.476	± 0.911	± 1.136			
2010	± 2.000	± 3.466	± 0.911	± 5.136			
3000	± 2.000	± 4.267	± 1.895	± 7.116			
4000	± 2.000	± 4.843	± 2.564	± 9.116			
5000	± 2.000	± 5.289	± 3.066	± 11.116			
6000	± 2.000	± 5.654	± 3.468	± 13.116			

TABLE 192

TITANIUM MONOXIDE IDEAL MOLECULAR GAS **OTi**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ti from 0° to 1950°K, Liquid Ti from 1950° to 3550°K, Gaseous Ti from 3550° to 6000°K, Gaseous O_2, Gaseous TiO.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.291	12.896	12.896	INFINITE
298.15	7.814	55.989	55.989	0.000	13.000	5.798	-4.250
300	7.821	56.037	55.989	0.014	12.996	5.753	-4.191
400	8.144	58.333	56.300	0.813	12.820	3.365	-1.838
500	8.405	60.179	56.897	1.641	12.634	1.023	-0.447
600	8.595	61.730	57.577	2.492	12.434	-1.281	0.467
700	8.730	63.065	58.268	3.358	12.217	-3.551	1.109
800	8.825	64.238	58.942	4.236	11.986	-5.788	1.581
900	8.893	65.281	59.589	5.122	11.740	-7.994	1.941
1000	8.941	66.221	60.206	6.014	11.478	-10.172	2.223
1100	8.977	67.075	60.793	6.910	11.201	-12.326	2.449
1155	8.992	67.513	61.102	7.404	11.042	-13.497	2.554
1155	8.992	67.513	61.102	7.404	10.092	-13.497	2.554
1200	9.003	67.857	61.349	7.809	9.960	-14.413	2.625
1300	9.022	68.578	61.878	8.711	9.656	-16.434	2.763
1400	9.038	69.248	62.381	9.614	9.336	-18.429	2.877
1500	9.050	69.872	62.859	10.518	9. 05	-20.400	2.972
1600	9.061	70.456	63.316	11.424	8.662	-22.350	3.053
1700	9.070	71.006	63.753	12.330	8.306	-24.278	3.121
1800	9.079	71.524	64.170	13.238	7.938	-26.183	3.179
1900	9.088	72.016	64.570	14.146	7.558	-28.068	3.228
1950	9.092	72.252	64.764	14.601	7.364	-29.002	3.250
1950	9.092	72.252	64.764	14.601	3.665	-29.002	3.250
2000	9.097	72.482	64.954	15.055	3.492	-29.838	3.260
2100	9.106	72.926	65.323	15.966	3.150	-31.496	3.278
2200	9.115	73.350	65.679	16.877	2.805	-33.139	3.292
2300	9.125	73.755	66.021	17.789	2.459	-34.765	3.303
2400	9.135	74.144	66.352	18.702	2.112	-36.376	3.312
2500	9.146	74.517	66.671	19.616	1.761	-37.974	3.320
2600	9.157	74.876	66.980	20.531	1.410	-39.555	3.325
2700	9.169	75.222	67.279	21.447	1.057	-41.126	3.329
2800	9.180	75.556	67.568	22.364	0.703	-42.678	3.331
2900	9.193	75.878	67.849	23.283	0.349	-44.221	3.332
3000	9.205	76.190	68.122	24.203	-0.008	-45.753	3.333
3100	9.217	76.492	68.388	25.124	-0.[illegible]	-47.275	3.333
3200	9.230	76.785	68.646	26.046	-0.724	-48.784	3.332
3300	9.243	77.069	68.897	26.970	-1.083	-50.277	3.330
3400	9.255	77.346	69.141	27.895	-1.442	-51.761	3.327
3500	9.268	77.614	69.380	28.821	-1.804	-53.239	3.324
3550	9.274	77.746	69.497	29.285	-1.984	-53.974	3.323
3550	9.274	77.746	69.497	29.285	-104.440	-53.974	3.323
3600	9.281	77.876	69.612	29.749	-104.626	-53.260	3.233
3700	9.293	78.130	69.839	30.677	-105.009	-51.828	3.061
3800	9.306	78.378	70.061	31.607	-105.405	-50.386	2.898
3900	9.318	78.620	70.277	32.538	-105.817	-48.934	2.742
4000	9.330	78.857	70.489	33.471	-106.240	-47.470	2.594
4100	9.342	79.087	70.696	34.404	-106.678	-45.995	2.452
4200	9.354	79.313	70.899	35.339	-107.128	-44.511	2.316
4300	9.365	79.533	71.097	36.275	-107.590	-43.012	2.186
4400	9.376	79.749	71.292	37.212	-108.065	-41.507	2.062
4500	9.387	79.960	71.482	38.150	-108.552	-39.992	1.942
4600	9.398	80.167	71.669	[illegible].090	-109.049	-38.460	1.827
4700	9.409	80.369	71.852	40.030	-109.559	-36.923	1.717
4800	9.419	80.568	72.032	40.971	-110.081	-35.372	1.610
4900	9.429	80.762	72.208	41.914	-110.612	-33.807	1.508
5000	9.439	80.953	72.382	42.857	-111.156	-32.240	1.409
5100	9.448	81.140	72.552	43.801	-111.712	-30.656	1.314
5200	9.458	81.324	72.719	44.747	-112.278	-29.063	1.221
5300	9.467	81.505	72.884	45.693	-112.857	-27.458	1.132
5400	9.476	81.682	73.045	46.640	-113.450	-25.842	1.046
5500	9.485	81.857	73.204	47.588	-114.057	-24.210	0.962
5600	9.493	82.028	73.361	48.537	-114.679	-22.580	0.881
5700	9.502	82.197	73.515	49.487	-115.318	-20.926	0.802
5800	9.510	82.362	73.666	50.438	-115.977	-19.262	0.726
5900	9.518	82.526	73.816	51.389	-116.659	-17.592	0.652
6000	9.526	82.686	73.963	52.341	-117.365	-15.908	0.579

15 June 1963 HLS

TITANIUM MONOXIDE (TiO) (IDEAL MOLECULAR GAS) gfw = 63.90

ΔH°_{f0} = 12.896 kcal gfw^{-1}

$\Delta H^{\circ}_{f298.15}$ = 13.0 kcal gfw^{-1}

Ground-State Configuration = $^{3}\pi$

$S^{\circ}_{298.15}$ = 55.989 cal deg K^{-1} gfw^{-1}

$H^{\circ}_{298.15} - H^{\circ}_{0}$ = 2.291 kcal gfw^{-1}

State	g	E	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e \times 10^5$	$D_e \times 10^6$
		cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}
$X^3\pi$	2	0	1008.6	4.61	0	0.5355	0.0031	0	0.603
	2	66.7	1008.6	4.61	0	0.5355	0.0031	0	0.603
	2	141.3	1008.6	4.61	0	0.5355	0.0031	0	0.603
$a^1\Delta$	2	581	1009.6	0.0	0	0.5362	0.0	0	0.604
$d^1\Sigma$	1	1708	1023.8	4.64	0	0.5490	0.00337	0	0.0
$b^1\pi$	2	10814	918.7	3.75	0	0.513	0.0029	0	0.0

Heat of Formation

Has been based on a preliminary analysis; a value of $\Delta H^{\circ}_{298.15}$ = 13.0 kcal gfw^{-1} is accepted. See volume 1, this study (section IVB30.4.1) for further references.

Heat Capacity and Entropy

Have been calculated by use of diatomic gas program. Energy levels are based on Herzberg,[1] Phillips,[2] and Pettersson and Lindgren.[3]

References

1. Herzberg, G., Spectra of Diatomic Molecules, Van Nostrand, New York (1950).
2. Phillips, J. G., Astrophys. J. 115, 567 (1952).
3. Pettersson, A. V. and B. Lindgren, Arkiv Fysik 22, 491 (1962).

TITANIUM MONOXIDE (TIO) (IDEAL MOLECULAR GAS) GFW = 63.90

SUMMARY OF UNCERTAINTY ESTIMATES

T °K	cal/°K gfw			Kcal/gfw			
	C°_{p}	S°_{T}	$-(F^{\circ}_{T} - H^{\circ}_{298})/T$	$H^{\circ}_{T} - H^{\circ}_{298}$	ΔH_f	ΔF_f	Log K_p
298.15	± 0.300	± 1.500	± 1.500	± 0.000	± 5.000		
1000	± 0.300	± 1.500	± 1.500	± 0.200			
2000	± 0.200	± 2.000	± 2.000	± 0.300			
3000	± 0.200	± 2.000	± 2.000	± 0.400			
4000	± 0.200	± 2.000	± 2.000	± 0.600			
5000	± 0.200	± 2.000	± 2.000	± 0.800			
6000	± 0.200	± 2.000	± 2.000	± 1.000			

TABLE 193

URANIUM MONOXIDE **IDEAL MOLECULAR GAS** **OU**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid U from 0° to 1406°K, Liquid U from 1406° to 4124°K, Gaseous U from 4124° to 6000°K; Gaseous O_2; Gaseous UO.

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-2.105	-11.346	-11.346	INFINITE
298.15	7.429	57.657	57.657	0.000	-11.800	-18.108	13.273
300	7.436	57.703	57.657	0.014	-11.804	-18.148	13.220
400	7.812	59.896	57.954	0.777	-12.081	-20.221	11.048
500	8.098	61.671	58.525	1.573	-12.382	-22.221	9.712
600	8.300	63.167	59.178	2.394	-12.726	-24.158	8.799
700	8.443	64.458	59.842	3.231	-13.134	-26.032	8.127
800	8.545	65.592	60.491	4.081	-13.629	-27.841	7.605
900	8.620	66.603	61.115	4.939	-14.229	-29.583	7.183
940	8.644	66.979	61.357	5.285	-14.503	-30.260	7.035
940	8.644	66.979	61.357	5.285	-15.188	-30.260	7.035
1000	8.676	67.514	61.710	5.804	-15.527	-31.210	6.821
1048	8.698	67.922	61.985	6.221	-15.798	-31.957	6.664
1048	8.698	67.922	61.985	6.221	-16.918	-31.957	6.664
1100	8.719	68.344	62.276	6.674	-17.160	-32.697	6.496
1200	8.753	69.104	62.814	7.548	-17.625	-34.089	6.208
1300	8.780	69.805	63.325	8.424	-18.092	-35.442	5.958
1400	8.801	70.457	63.811	9.304	-18.559	-36.759	5.738
1406	8.802	70.494	63.840	9.356	-18.588	-36.839	5.726
1406	8.802	70.494	63.840	9.356	-23.288	-36.839	5.726
1500	8.819	71.065	64.275	10.185	-23.728	-37.730	5.497
1600	8.833	71.034	64.717	11.067	-24.200	-38.647	5.279
1700	8.845	72.170	65.140	11.951	-24.672	-39.535	5.082
1800	8.855	72.676	65.545	12.836	-25.147	-40.397	4.905
1900	8.864	73.155	65.933	13.722	-25.623	-41.232	4.743
2000	8.872	73.610	66.305	14.609	-26.101	-42.038	4.593
2100	8.879	74.043	66.664	15.496	-26.582	-42.826	4.457
2200	8.884	74.456	67.009	16.385	-27.063	-43.587	4.330
2300	8.889	74.851	67.341	17.273	-27.548	-44.328	4.212
2400	8.893	75.229	67.662	18.162	-28.035	-45.046	4.102
2500	8.897	75.593	67.972	19.052	-28.524	-45.746	3.999
2600	8.900	75.942	68.272	19.942	-29.015	-46.425	3.902
2700	8.903	76.278	68.562	20.832	-29.510	-47.085	3.811
2800	8.906	76.601	68.843	21.722	-30.005	-47.724	3.725
2900	8.909	76.914	69.116	22.613	-30.503	-48.350	3.644
3000	8.911	77.216	69.381	23.504	-31.003	-48.956	3.566
3100	8.913	77.508	69.639	24.395	-31.506	49.547	3.493
3200	8.915	77.791	69.889	25.287	-32.010	-50.122	3.423
3300	8.916	78.066	70.133	26.178	-32.516	-50.681	3.356
3400	8.918	78.332	70.370	27.070	-33.024	-51.221	3.292
3500	8.919	78.590	70.601	27.962	-33.53.	-51.747	3.231
3600	8.920	78.842	70.827	28.854	-34.046	-52.262	3.173
3700	8.922	79.086	71.047	29.746	-34.560	-52.763	3.116
3800	8.923	79.324	71.261	30.638	-35.075	-53.245	3.062
3900	8.924	79.556	71.471	31.530	-35.593	-53.715	3.010
4000	8.925	79.782	71.676	32.423	-36.111	-54.174	2.960
4100	8.925	80.002	71.876	33.315	-36.632	-54.620	2.911
4123.63	8.926	80.053	71.923	33.526	-36.755	-54.723	2.900
4123.63	8.926	80.053	71.923	33.526	-143.656	-54.727	2.900
4200	8.926	80.217	72.072	34.208	-144.143	-53.069	2.761
4300	8.927	80.427	72.264	35.100	-144.787	-50.896	2.587
4400	8.928	80.632	72.452	35.993	-145.439	-48.703	2.419
4500	8.928	80.833	72.636	36.886	-146.096	-46.479	2.258
4600	8.929	81.029	72.817	37.779	-146.761	-44.281	2.104
4700	8.930	81.221	72.993	38.672	-147.431	-42.040	1.955
4800	8.930	81.409	73.167	39.565	-148.110	-39.791	1.812
4900	8.931	81.593	73.337	40.458	-148.794	-37.532	1.674
5000	8.931	81.774	73.504	41.351	-149.487	-35.250	1.541
5100	8.932	81.951	73.668	42.244	-150.187	-32.960	1.412
5200	8.932	82.124	73.829	43.137	-150.894	-30.650	1.288
5300	8.932	82.294	73.987	44.030	-151.609	-28.333	1.168
5400	8.933	82.461	74.142	44.924	-152.334	-25.997	1.052
5500	8.933	82.625	74.295	45.817	-153.069	-23.650	0.940
5600	8.933	82.786	74.445	46.710	-153.816	-21.289	0.831
5700	8.934	82.944	74.593	47.604	-154.575	-18.914	0.725
5800	8.934	83.100	74.738	48.497	-155.352	-16.518	0.622
5900	8.934	83.252	74.881	49.390	-156.146	-14.119	0.523
6000	8.935	83.403	75.022	50.284	-156.960	-11.704	0.426

15 June 1963 MBP

URANIUM MONOXIDE (UO) (IDEAL MOLECULAR GAS) gfw = 254.07

ΔH_{f0} = - 11.346 kcal gfw^{-1}

$\Delta H^{\circ}_{f298.15}$ = -11.8 ± 10 kcal gfw^{-1}

Ground State Configuration $^{1}\Sigma$

$S^{\circ}_{298.15}$ = 57.7 cal deg K^{-1} gfw^{-1}

$H^{\circ}_{298.15} - H^{\circ}_{0}$ = 2.105 kcal gfw^{-1}

Spectroscopic Constants
cm^{-1}
ω_e = 920
B_e = 0.2924

Heat of Formation

Calculated from the data of DeMaria, Burns, Drowart, and Inghram.[1]

Heat Capacity and Entropy

Calculated using the diatomic gas program and the constants listed above.

Reference

1. DeMaria. G., P. Burns, J. Drowart, and M. Inghram, J. Chem. Phys. 32, 1373 (1960).

TABLE 194

TUNGSTEN MONOXIDE IDEAL MOLECULAR GAS **OW**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid W from 0° to 3650°K, Liquid W from 3650° to 5891°K, Gaseous W from 5891° to 6000°K; Gaseous O_2; Gaseous WO.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.122	97.510	97.510	INFINITE
298.15	7.601	56.597	56.597	0.000	97.400	90.166	-66.090
300	7.609	56.643	56.597	0.014	97.396	90.121	-65.650
400	7.990	58.888	56.900	0.795	97.234	87.730	-47.931
500	8.252	60.701	57.485	1.608	97.081	85.362	-37.310
600	8.428	62.222	58.151	2.443	96.931	83.044	-30.247
700	8.547	63.531	58.828	3.292	96.777	80.728	-25.203
800	8.631	64.678	59.489	4.151	96.616	78.461	-21.433
900	8.691	65.698	60.123	5.017	96.446	76.184	-18.499
1000	8.736	66.616	60.728	5.889	96.273	73.962	-16.164
1100	8.770	67.450	61.301	6.764	96.088	71.717	-14.248
1200	8.796	68.215	61.846	7.642	95.896	69.535	-12.663
1300	8.817	68.920	62.363	8.523	95.689	67.319	-11.317
1400	8.834	69.574	62.855	9.405	95.466	65.145	-10.169
1500	8.847	70.183	63.324	10.290	95.230	62.988	-9.177
1600	8.859	70.755	63.771	11.175	94.973	60.843	-8.310
1700	8.868	71.292	64.197	12.061	94.701	58.721	-7.549
1800	8.876	71.799	64.606	12.948	94.410	56.614	-6.873
1900	8.883	72.279	64.997	13.836	94.104	54.521	-6.271
2000	8.888	72.735	65.373	14.725	93.780	52.444	-5.731
2100	8.893	73.169	65.734	15.614	93.439	50.387	-5.244
2200	[illegible]	73.583	66.081	16.503	93.080	48.345	-4.802
2300	8.901	73.978	66.416	17.393	92.705	46.320	-4.401
2400	8.905	74.357	66.739	18.284	92.311	44.314	-4.035
2500	8.908	74.721	67.051	19.174	91.900	42.323	-3.700
2600	8.910	75.070	67.353	20.065	91.472	40.347	-3.391
2700	8.913	75.407	67.645	20.956	91.028	38.386	-3.107
2800	8.915	75.731	67.928	21.[illegible]48	90.565	36.445	-2.845
2900	8.917	76.044	68.202	22.739	90.085	34.525	-2.602
3000	8.918	76.346	68.469	23.631	89.588	32.613	-2.376
3100	8.920	76.638	68.728	24.523	89.075	30.724	-2.166
3200	8.921	76.922	68.979	25.415	88.543	28.854	-1.971
3300	8.922	77.196	69.224	26.307	87.995	26.994	-1.788
3400	8.924	77.463	69.463	27.200	87.431	25.153	-1.617
3500	8.925	77.721	69.695	28.092	86.848	23.328	-1.457
3600	8.926	77.973	69.921	28.985	86.249	21.528	-1.307
3650	8.927	78.095	70.032	29.431	85.944	20.633	-1.235
3650	8.927	78.095	70.032	29.431	77.549	20.633	-1.235
3700	8.927	78.217	70.142	29.877	77.250	19.851	-1.172
3800	8.927	78.455	70.358	30.770	76.65[illegible]	18.312	-1.053
3900	8.928	78.687	70.569	31.663	76.049	16.774	-0.940
4000	8.929	78.913	70.774	32.555	75.445	15.276	-0.835
4100	8.930	79.134	70.976	33.448	74.840	13.768	-0.734
4200	8.930	79.349	71.172	34.341	74.233	12.247	-0.637
4300	8.931	79.559	71.365	35.234	73.624	10.827	-0.550
4400	8.931	79.764	71.554	36.128	73.014	9.372	-0.465
4500	8.932	79.965	71.738	37.021	72.402	7.929	-0.385
4600	8.932	80.161	71.919	37.914	71.787	6.509	-0.309
4700	8.933	80.353	72.097	38.807	71.169	5.095	-0.237
4800	8.933	80.542	72.271	39.700	70.549	3.691	-0.168
4900	8.933	80.726	72.441	40.594	69.926	2.[illegible]13	-0.103
5000	8.934	80.906	72.609	41.487	69.299	0.[illegible]49	-0.041
5100	8.934	81.083	72.773	42.[illegible]81	68.668	-0.423	0.018
5200	8.935	81.257	72.935	43.274	68.031	-1.768	0.074
5300	8.935	81.427	73.093	44.167	67.387	-3.101	0.128
5400	8.935	81.594	73.249	45.061	66.737	-4.417	0.179
5500	8.935	81.758	73.402	45.954	66.078	-5.731	0.228
5600	8.936	81.919	73.553	46.848	65.408	-7.034	0.274
5700	8.936	82.077	73.701	47.742	64.726	-8.322	0.319
5800	8.936	82.232	73.847	48.635	64.027	-9.593	0.361
5891	8.936	82.371	73.977	49.449	63.376	-10.739	0.398
5891	8.936	82.371	73.977	49.449	-128.889	-10.739	0.398
5900	8.936	82.385	73.990	49.529	-128.951	-10.567	0.391
6000	8.937	82.535	74.137	50.422	-129.663	-8.550	0.311

May 1962 CHW

TUNGSTEN MONOXIDE (WO) (IDEAL MOLECULAR GAS) gfw = 199.86

$\Delta H^{\circ}_{f0} = 97.510$ kcal gfw^{-1}

$\Delta H^{\circ}_{f298.15} = 97.400$ kcal gfw^{-1}

Ground State Configuration = $^1\Sigma$

$S^{\circ}_{298.15} = 56.597$ cal degK^{-1} gfw^{-1}

$H^{\circ}_{298.15} - H^{\circ}_0 = 2.122$ kcal gfw^{-1}

State	g	E	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e \times 10^5$	$D_e \times 10^6$
		cm^{-1}							
$^1\Sigma$	1	0.0	803	-	-	0.36149	-	-	-

Heat of Formation

Based on work of DeMaria and co-workers.[1]

Heat Capacity and Entropy

Calculated using estimated constants.[2]

References

1. De Maria, G. et al, J. Chem. Phys. 32, 1373 (1960).
2. Barriault, R. J. et al, ASD TR 61-260, (May 1962), Pt. 1.

YTTRIUM MONOXIDE

IDEAL MOLECULAR GAS

OY

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Y from 0° to 1803°K. Liquid Y from 1803° to 3605°K. Gaseous Y from 3605° to 6000°K; Gaseous O_2; Gaseous YO.

T, °K	cal/°K gfw C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	Kcal/gfw $H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-2.115	-11.800	-11.800	INFINITE
298.15	7.537	55.883	55.883	0.000	-12.148	-18.334	13.439
300	7.545	55.930	55.883	0.014	-12.152	-18.373	13.384
400	7.932	58.156	56.184	0.789	-12.375	-20.412	11.152
500	8.210	59.958	56.764	1.597	-12.592	-22.396	9.789
600	8.401	61.473	57.426	2.428	-12.814	-24.337	8.864
700	8.535	62.778	58.100	3.275	-13.046	-26.239	8.192
800	8.630	63.925	58.758	4.134	-13.294	-28.108	7.678
900	8.701	64.945	59.389	5.000	-13.561	-29.942	7.271
1000	8.755	65.865	59.992	5.873	-13.845	-31.747	6.938
1100	8.797	66.701	60.564	6.751	-14.147	-33.523	6.660
1200	8.830	67.468	61.108	7.632	-14.469	-35.270	6.423
1300	8.858	68.176	61.625	8.517	-14.808	-36.990	6.218
1400	8.881	68.834	62.117	9.404	-15.169	-38.685	6.039
1500	8.900	69.447	62.585	10.293	-15.549	-40.350	5.879
1600	8.918	70.022	63.032	11.184	-15.951	-41.990	5.735
1700	8.933	70.563	63.459	12.076	-16.373	-43.605	5.606
1758	8.940	70.859	63.696	12.594	-16.679	-44.527	5.535
1758	8.940	70.859	63.696	12.594	-17 318	-44.527	5.535
1800	8.946	71.074	63.868	12.970	-17.981	-45.166	5.484
1803	8.946	71.088	63.880	12.997	-17.992	-45.211	5.480
1803	8.946	71.088	63.880	12.997	-20.724	-45.211	5.480
1900	8.959	71.558	64.261	13.865	-21.289	-46.516	5.350
2000	8.972	72.018	64.637	14.762	-21.872	-47.826	5.226
2100	8.984	72.456	64.999	15.660	-22.458	-49.109	5.111
2200	8.997	72.874	65.348	16.559	-23.044	-50.365	5.003
2300	9.010	73.275	65.684	17.459	-23.632	-51.594	4.902
2400	9.025	73.659	66.008	18.361	-24.222	-52.798	4.808
2500	9.041	74.027	66.322	19.264	-24.813	-53.977	4.718
2600	9.059	74.382	66.625	[illegible].169	-25.404	-55.130	4.634
2700	9.078	74.725	66.919	21.076	-25.997	-56.265	4.554
2800	9.100	75.0[illegible]	67.203	21.985	-26.589	-57.374	4.478
2900	9.124	75.375	67.480	22.896	-27.182	-58.462	4.406
3000	9.151	75.6[illegible]	67.748	23.810	-27.774	-59.531	4.337
3100	9.181	75.986	68.009	24.727	-28.367	-60.578	4.271
3200	9.213	76.278	68.26[illegible]	25.646	-28.959	-61.609	4.207
3300	9.249	76.562	68.510	26.569	-29.5[illegible]8	-62.621	4.147
3400	9.287	76.839	68.751	27.496	-30.1[illegible]	-63.615	4.089
3500	9.328	77.108	68.986	28.427	-30.7[illegible]	-64.590	4.033
3600	9.372	77.372	69.216	29.362	-31.307	-65.552	3.979
3604.66	9.374	77.384	69.226	29.406	-31.334	-65.596	3.977
3604.66	9.374	77.384	69.226	29.406	-118.512	-65.596	3.977
3700	9.418	77.629	69.440	30.301	-118.358	-64.207	3.792
3800	9.467	77.861	69.659	31.246	-118.741	-62.739	3.608
3900	9.519	78.128	69.873	32.195	-119.147	-61.259	3.433
4000	9.573	78.370	70.083	33.150	-119.571	-59.774	3.266
4100	9.629	78.607	70.288	34.110	-120.014	-58.273	3.106
4200	9.687	78.840	70.489	35.076	-120.476	-56.760	2.953
4300	9.747	79.069	70.686	36.047	-120.954	-55.234	2.807
4400	9.809	79.294	70.879	37.025	-121.448	-53.702	2.667
4500	9.872	79.516	71.069	38.010	-121.955	-52.162	2.533
4600	9.936	79.734	71.255	39.000	-122.477	-50.599	2.404
4700	10.002	79.948	71.438	39.997	-123.010	-4[illegible].034	2.280
4800	10.068	80.160	71.618	41.001	-123.555	-4[illegible].459	2.161
4900	10.135	80.369	71.795	.012	-124.108	-45.867	2.046
5000	10.203	80.574	71.968	43.029	-124.672	-44.258	1.934
5100	10.271	80.777	72.140	44.053	-125.244	-42.656	1.828
5200	10.339	80.978	72.308	45.085	-125.823	-41.029	1.724
5300	10.407	81.176	72.474	46.123	-126.410	-39.393	1.624
5400	10.475	81.372	72.637	47.168	-127.005	-37.744	1.528
5500	10.543	81.56[illegible]	72.798	48.219	-127.609	-36.087	1.434
5600	10.610	81.756	72.957	49.278	-128.220	-34.422	1.343
5700	10.677	81.945	73.113	50.344	-128.936	-32.742	1.255
5800	10.743	82.132	73.267	51.416	-129.474	-31.041	1.170
5900	10.808	82.317	73.420	52.495	-130.1[illegible]	-29.346	1.087
6000	10.872	82.500	73.570	5[illegible].581	-130.785	-27.628	1.006

15 March 1963

MG

ΔH^o_{f0} = -11.8 Kcal gfw^{-1}

Ground State Configuration $^2\Sigma$

$H^o_{298.15} - H^o_0$ = 2.115 Kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = -12.148 Kcal gfw^{-1}

$S^o_{298.15}$ = 55.883 cal deg K^{-1} gfw^{-1}

State	g	E (cm^{-1})	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e \times 10^5$	$D_e \times 10^7$
$^2\Sigma$	2	0.0	852.5	2.45	0.0273	0.3889	0.0016	0.0	3.2
A $^2\Pi$	2	16294.72	812.7	2.80	0.0	0.3867	0.0019	0.0	3.5
A $^2\Pi$	2	16722.75	808.9	2.96	0.0	0.3867	0.0019	0.0	3.5
B $^2\Sigma$	2	20741.92	765.03	7.75	0.0	0.3742	0.0039	0.0	3.9

Heat of Formation

From a study of vaporization of Y_2O_3 by Walsh *et al.*[1]

Heat Capacity and Entropy

Calculated on diatomic gas program.

Reference

1. Walsh, P. N., H. W. Goldstein and D. White, J. Am. Ceram. Soc. 43, 229 (1960).

ZIRCONIUM MONOXIDE — IDEAL MOLECULAR GAS — OZr

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Zr from 0° to 2125°K, Liquid Zr from 2125° to 4644°K, Gaseous Zr from 4644° to 6000°K; Gaseous O_2, Gaseous ZrO.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.335	21.116	21.116	INFINITE
298.15	8.632	57.055	57.055	0.000	21.100	14.165	-10.382
300	8.636	57.108	57.055	0.016	21.098	14.122	-10.287
400	8.829	59.621	57.396	0.890	20.986	11.812	-6.453
500	8.948	61.605	58.047	1.779	20.837	9.535	-4.167
600	9.018	63.243	58.780	2.678	20.657	7.291	-2.656
700	9.058	64.637	59.520	3.582	20.449	5.079	-1.586
800	9.079	65.848	60.237	4.489	20.215	2.899	-0.792
900	9.090	66.918	60.921	5.397	19.957	0.750	-0.182
1000	9.096	67.876	61.569	6.307	19.677	-1.368	0.299
1100	9.098	68.743	62.183	7.216	19.375	-3.460	0.687
1135	9.099	69.028	62.389	7.535	19.266	-4.184	0.806
1135	9.099	69.028	62.389	7.535	18.351	-4.184	0.806
1200	9.099	69.535	62.763	8.126	18.152	-5.470	0.996
1300	9.100	70.263	63.312	9.036	17.843	-7.425	1.248
1400	9.101	70.937	63.833	9.946	17.[illegible]31	-9.358	1.461
1500	9.102	71.565	64.328	10.856	17.[illegible]16	-11.268	1.642
1600	9.105	72.153	64.799	11.767	16.899	-13.157	1.797
1700	9.108	72.705	65.248	12.677	16.577	-15.025	1.932
1800	9.112	73.226	65.677	13.588	16.254	-16.875	2.049
1900	9.118	73.719	66.087	14.500	15.929	-18.706	2.152
2000	9.124	74.186	66.480	15.412	15.601	-20.520	2.242
2100	9.130	74.632	66.858	16.325	15.271	-22.319	2.323
2125	9.132	74.740	66.950	16.553	15.189	-22.764	2.341
2125	9.132	74.740	66.950	16.553	10.288	-22.764	2.341
2200	9.138	75.057	67.221	17.238	10.031	-23.926	2.377
2300	9.146	75.463	67.571	18.152	9.688	-25.465	2.420
2400	9.155	75.853	67.908	19.067	9.342	-26.985	2.457
2500	9.164	76.227	68.233	19.983	8.993	-28.491	2.491
2600	9.173	76.586	68.548	20.900	8.644	-29.983	2.520
2700	9.183	76.933	68.852	21.818	8.293	-31.465	2.547
2800	9.192	77.267	69.147	22.737	7.942	-32.932	2.570
2900	9.202	77.590	69.432	23.656	7.586	-34.381	2.591
3000	9.212	77.902	69.710	24.577	7.231	-35.826	2.610
3100	9.222	78.204	69.979	2[illegible].499	6.875	-37.253	2.626
3200	9.232	78.497	70.241	26.421	6.516	-38.674	2.641
3300	9.242	78.782	70.495	27.345	6.157	-40.079	2.654
3400	9.251	79.058	70.743	28.270	5.798	-41.475	2.666
3500	9.261	79.326	70.985	29.195	5.435	-42.861	2.676
3600	9.270	79.588	71.220	30.122	5.073	-44.235	2.685
3700	9.280	79.842	71.450	31.049	4.710	-45.600	2.693
3800	9.289	80.090	71.674	31.978	4.347	-46.956	2.700
3900	9.298	80.331	71.893	32.907	3.981	-48.299	2.706
4000	9.307	80.567	72.108	33.837	3.615	-49.638	2.712
4100	9.315	80.797	72.317	34.768	3.248	-50.966	2.717
4200	9.324	81.022	72.522	35.700	2.880	-52.287	2.721
4300	9.332	81.242	72.722	36.633	2.512	-53.591	2.724
4400	9.340	81.456	72.919	37.567	2.142	-54.897	2.727
4500	9.348	81.667	73.111	38.501	1.770	-56.187	2.729
4600	9.356	81.873	73.299	39.436	1.397	-57.468	2.730
4644.05	9.360	81.962	73.381	39.849	1.234	-58.030	2.731
4644.05	9.360	81.962	73.381	[illegible]849	-134.220	-58.030	2.731
4700	9.364	82.074	73.484	40.372	-134.485	-57.113	2.656
4800	9.371	82.272	73.666	41.309	-134.963	-55.467	2.525
4900	9.379	82.465	73.844	42.247	-135.448	-53.804	2.400
5000	9.386	82.655	74.018	43.185	-135.942	-52.130	2.278
5100	9.393	82.842	74.190	44.124	-136.444	-50.458	2.162
5200	9.401	83.024	74.358	45.064	-136.955	-48.762	2.049
5300	9.408	83.204	74.524	46.004	-137.476	-47.066	1.941
5400	9.414	83.380	74.687	46.945	-138.007	-45.358	1.836
5500	9.421	83.554	74.847	47.887	-138.549	-43.638	1.734
5600	9.428	83.724	75.004	48.829	-139.105	-41.903	1.635
5700	9.435	83.891	75.159	49.772	-139.676	-40.164	1.540
5800	9.441	84.056	75.312	50.716	-140.264	-38.417	1.448
5900	9.448	84.218	75.462	51.661	-140.871	-36.655	1.358
6000	9.454	84.377	75.610	52.606	-141.502	-34.880	1.270

15 June 1963 HLS

ZIRCONIUM MONOXIDE (ZrO) (IDEAL MOLECULAR GAS) gfw = 107.22

ΔH°_{f0} = 21.116 kcal gfw^{-1}

$\Delta H^{\circ}_{f298.15}$ = 21.1 kcal gfw^{-1}

Ground-State Configuration = $^{3}\Delta$

$S^{\circ}_{298.15}$ = 57.055 cal deg K^{-1} gfw^{-1}

$H^{\circ}_{298.15} - H^{\circ}_{0}$ = 2.335 kcal gfw^{-1}

State	g	E	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e \times 10^5$	$D_e \times 10^6$
		cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}	cm^{-1}
$c^1\Sigma$	1	9171.2	938.1	1.80	---	0.3951	0.0019	---	0.35
$a^1\Sigma$	1	1320.3	978.07	5.04	---	0.4241	0.0023	---	0.33
$x^3\Delta$	2	605.1							
	2	297.2	936.5	3.47	---	0.4156	0.0021	---	0.32
	2	0							

Heat of Formation

No analysis has been performed; data of JANAF Tables[1] have been accepted temporarily.

Heat Capacity and Entropy

Have been calculated; have used above energy levels. See volume 1, this study (section IVB35.4.1) for details.

Reference

1. JANAF, Thermochemical Tables (30 September 1961).

ZIRCONIUM MONOXIDE (ZrO) (IDEAL MOLECULAR GAS) GFW = 107.22

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^{\circ}_T - H^{\circ}_{298})/T$ (cal/°K gfw)	$H^{\circ}_T - H^{\circ}_{298}$ (Kcal/gfw)	ΔH°_f (Kcal/gfw)	ΔF°_f (Kcal/gfw)	Log K_p
298.15	± 0.200	± 1.000	± 1.000	± 0.000	±5 000		
1000	± 0.500	± 1.700	± 1.200	± 0.500			
2000	± 0.500	± 2.000	± 1.600	± 1.000			
3000	± 0.500	± 2.200	± 1.800	± 1.300			
4000	± 0.500	± 2.300	± 1.900	± 1.600			
5000	± 0.500	± 2.400	± 2.000	± 1.900			
6000	± 0.500	± 2.400	± 2.000	± 2.000			

TABLE 197

OXYGEN

REFERENCE STATE

O_2

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p :
Gaseous Diatomic O_2 from 0° to 6000°K.

T, °K	cal/°K gfw C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	Kcal/gfw $H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-2.075			
298.15	7.021	49.007	49.007	0.000			
300	7.024	49.051	49.007	0.013			
400	7.196	51.092	49.284	0.723			
500	7.431	52.723	49.814	1.454			
600	7.670	54.099	50.417	2.210			
700	7.884	55.298	51.030	2.987			
800	8.064	56.363	51.631	3.785			
900	8.213	57.321	52.211	4.599			
1000	8.336	58.193	52.767	5.427			
1100	8.439	58.993	53.297	6.266			
1200	8.527	[illegible].731	53.803	7.114			
1300	8.604	60.417	54.285	7.971			
1400	8.674	61.057	54.746	8.835			
1500	8.738	61.657	55.187	9.705			
1600	8.799	62.223	55.609	10.582			
1700	8.858	62.759	56.014	11.465			
1800	8.915	63.267	56.403	12.354			
1900	8.972	63.750	56.777	13.248			
2000	9.028	64.212	57.138	14.148			
2100	9.083	64.654	57.485	15.054			
2200	9.138	65.077	57.821	15.965			
2300	9.193	65.485	58.145	16.881			
2400	9.246	65.877	58.459	17.803			
2500	9.299	66.256	58.763	18.731			
2600	9.351	66.622	59.059	19.663			
2700	9.402	66.975	59.345	20.601			
2800	9.451	67.318	59.624	21.543			
2900	9.499	67.651	59.895	2[illegible].491			
3000	9.546	67.974	60.159	23.443			
3100	9.591	68.288	60.417	24.400			
3200	9.635	68.593	60.667	25.362			
3300	9.677	68.890	60.912	26.327			
3400	9.718	69.180	61.151	27.297			
3500	9.758	69.462	61.385	28.271			
3600	9.796	69.738	61.613	29.249			
3700	9.833	70.007	61.836	30.230			
3800	9.869	70.269	62.055	31.215			
3900	9.905	70.526	62.269	3[illegible].204			
4000	9.940	70.778	62.479	33.196			
4100	9.976	71.024	62.684	34.192			
4200	10.012	71.265	62.886	35.192			
4300	10.049	71.501	63.084	36.195			
4400	10.088	[illegible].733	63.278	37.203			
4500	10.130	71.960	63.468	38.214			
4600	10.176	72.184	63.656	39.230			
4700	10.226	72.404	63.840	40.251			
4800	10.283	72.620	64.021	41.278			
4900	10.347	72.834	54.199	42.311			
5000	10.421	73.044	64.374	43.35[illegible]			
5100	10.506	73.252	64.546	44.402			
5200	10.607	73.459	64.716	45.462			
5300	10.724	73.663	64.883	[illegible].535			
5400	10.863	73.867	65.048	4[illegible].623			
5500	11.027	74.070	65.211	48.728			
5600	11.222	74.274	65.371	49.855			
5700	11.453	74.479	65.530	51.007			
5800	11.727	74.685	65.687	52.191			
5900	12.052	74.895	65.842	53.412			
6000	12.439	75.109	65.996	54.677			

May 1962 RCF

OXYGEN (O_2) (REFERENCE STATE) gfw = 32.000

ΔH°_{f0} = 0.0 kcal gfw^{-1}

$\Delta H^\circ_{f298.15}$ = 0.0 kcal gfw^{-1}

Ground State Configuration = $^3\Sigma_g^-$

$S^\circ_{298.15}$ = 49.007 cal deg K^{-1} gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 2.075 kcal gfw^{-1}

State	g	E (cm^{-1})	ω_e	$\omega_e x_e$	$\omega_e y_e$	B_e	α_e	$\gamma_e \times 10^5$	$D_e \times 10^6$
X $^3\Sigma_g^-$	3	-0.244	1580.1622	12.07	.0546	1.44531	0.01579	-	4.96
a $^1\Delta_g$	2	7882.36	1509.1	12.9	-	1.426	0.0171	-	5.1
b $^1\Sigma_g^+$	1	13120.917	1432.507	13.9406	-.01075	1.40007	0.01817	-4.3	5.36
A $^3\Sigma_u^+$	3	35008.0	801.	15.0	-	0.91	0.015	-	3.4
$^1\Sigma_u^-$	7	36212.8	650.41	17.03	-0.106	0.826	0.0205	-83.0	5.3
B $^3\Sigma_u^-$	3	49357.6	709.4	8.0	-0.375	0.819	0.011	-	4.4

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Calculated on diatomic gas-computer program, using above spectroscopic constants. Complete details of data used given by Barriault *et al*[1].

Reference

1. Barriault, R. J. *et al*, ASD TR 61-260 (May 1962), Pt. 1.

OXYGEN (O_2) (REFERENCE STATE) GFW = 32.000

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
298.15	±0.000	±0.003	±0.003	±0.000			
1000	±0.001	±0.004	±0.004	±0.001			
2000	±0.002	±0.005	±0.004	±0.002			
3000	±0.005	±0.007	±0.004	±0.005			
4000	±0.014	±0.009	±0.006	±0.014			
5000	±0.089	±0.018	±0.007	±0.057			
6000	±0.673	±0.081	±0.013	±0.407			

TABLE 198

OSMIUM DIOXIDE — IDEAL MOLECULAR GAS — O_2Os

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Os from 0° to 3290°K, Liquid Os from 3290° to 5270°K, Gaseous Os from 5270° to 6000°K; Gaseous O2; Gaseous OsO_2.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.849	17.836	17.836	INFINITE
298.15	11.914	61.455	61.455	0.000	17.400	16.014	-11.738
300	11.934	61.529	61.456	0.022	17.398	16.005	-11.659
400	12.835	65.095	61.936	1.264	17.330	15.553	-8.497
500	13.422	68.026	62.869	2.579	17.306	15.113	-6.606
600	13.805	70.510	63.941	3.941	17.294	14.675	-5.345
700	14.063	72.659	65.036	5.336	17.286	14.240	-4.446
800	14.242	74.549	66.110	6.751	17.268	13.805	-3.771
900	14.371	76.234	67.143	8.182	17.241	13.373	-3.247
1000	14.467	77.754	68.129	9.624	17.203	12.947	-2.829
1100	14.539	79.136	69.068	11.075	17.153	12.524	-2.488
1200	14.595	80.403	69.961	12.532	17.092	12.104	-2.204
1300	14.639	81.573	70.809	13.993	17.017	11.692	-1.965
1400	14.674	82.660	71.617	15.459	16.931	11.286	-1.762
1500	14.703	83.673	72.388	16.928	16.834	10.885	-1.586
1600	14.727	84.623	73.123	18.400	16.723	10.491	-1.433
1700	14.747	85.516	73.826	19.873	16.599	10.107	-1.299
1800	14.764	86.360	74.499	21.349	16.463	9.728	-1.181
1900	14.778	87.158	75.145	22.826	16.314	9.357	-1.076
2000	14.790	87.917	75.764	24.304	16.152	8.998	-0.983
2100	14.800	88.638	76.360	25.784	15.976	8.645	-0.900
2200	14.810	89.327	76.934	27.264	15.787	8.301	-0.825
2300	14.818	89.986	77.487	28.746	15.586	7.963	-0.757
2400	14.825	90.616	78.021	30.228	15.370	7.637	-0.695
2500	14.831	91.222	78.537	31.711	15.141	7.318	-0.640
2600	14.836	91.804	79.037	33.194	14.898	7.010	-0.589
2700	14.841	92.364	79.520	34.678	14.642	6.711	-0.543
2800	14.846	92.903	79.988	36.162	14.373	6.424	-0.501
2900	14.850	93.424	80.443	37.647	14.090	6.142	-0.463
3000	14.853	93.928	80.884	39.132	13.795	5.874	-0.428
3100	14.856	94.415	81.312	40.618	13.486	5.620	-0.396
3200	14.859	94.887	81.729	42.103	13.163	5.368	-0.367
3290	14.862	95.298	82.094	43.440	12.862	5.155	-0.342
3290	14.862	95.298	82.094	43.440	5.295	5.155	-0.342
3300	14.862	95.344	82.135	43.589	5.258	5.154	-0.341
3400	14.864	95.788	82.530	45.076	4.375	5.157	-0.331
3500	14.867	96.219	82.915	46.562	4.4[illegible]7	5.171	-0.323
3600	14.869	96.637	83.290	48.049	4.0[illegible]	5.196	-0.315
3700	14.871	97.045	83.657	49.536	3.702	5.231	-0.309
3800	14.872	97.441	84.014	51.023	3.304	5.282	-0.304
3900	14.874	97.828	84.363	52.511	2.903	5.337	-0.299
4000	14.875	98.204	84.705	53.998	2.498	5.404	-0.295
4100	14.877	98.572	85.039	55.486	2.090	5.481	-0.292
4200	14.878	98.930	85.365	56.973	1.677	5.573	-0.290
4300	14.879	99.280	85.685	58.461	1.262	5.670	-0.288
4400	14.881	99.672	85.998	59.949	0.842	5.775	-0.287
4500	14.882	99.957	86.304	61.437	0.419	5.893	-0.286
4600	14.883	100.284	86.604	62.926	-0.008	6.029	-0.286
4700	14.883	100.604	86.899	64.414	-0.441	6.162	-0.287
4800	14.884	100.917	87.188	65.902	-0.880	6.307	-0.287
4900	14.885	101.224	87.471	67.391	-1.324	6.463	-0.288
5000	14.886	101.525	87.749	68.879	-1.777	6.630	-0.290
5100	14.887	101.820	88.022	70.368	-2.238	6.802	-0.291
5200	14.887	102.109	88.290	71.857	-2.709	6.990	-0.294
5269.57	14.888	102.307	88.475	72.899	-3.044	7.113	-0.295
5269.57	14.888	102.307	88.475	72.899	-179.445	7.113	-0.295
5300	14.888	102.392	88.554	73.345	-179.588	8.199	-0.338
5400	14.889	102.671	88.813	74.834	-180.066	11.752	-0.476
5500	14.889	102.944	89.067	76.323	-180.565	15.151	-0.602
5600	14.890	103.212	89.317	77.812	-181.088	18.878	-0.737
5700	14.890	103.476	89.563	79.301	-181.639	22.462	-0.861
5800	14.891	103.735	89.805	80.790	-182.225	26.054	-0.982
5900	14.891	103.989	90.044	82.279	-182.850	29.654	-1.098
6000	14.892	104.240	90.278	83.768	-183.521	33.270	-1.212

15 September 1962 CHW

OSMIUM DIOXIDE (OsO_2) (IDEAL MOLECULAR GAS) gfw = 222.2

ΔH^o_{f0} = 17.836 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 17.400 kcal gfw^{-1}

Point Group = $D_{\infty v}$

$S^o_{298.15}$ = 61.455 cal deg K^{-1}gfw^{-1}

$H^o_{298.15}-H^o_0$ = 2.849 kcal gfw^{-1}

Vibrational Levels and Multiplicities

ω, cm^{-1}	ω, cm^{-1}
764 (1)	825 (1)
215 (2)	

Bond lengths and angles:

Os-O distance = 185 Å

$\sigma = 2$

O-Os-O angle = 180°

Heat of Formation

Estimated from Brewer et al data.[1]

Heat Capacity and Entropy

Determined from the estimated spectroscopic data. See volume 1, this study (section IVB18.4.2) for details.

Reference

1. Brewer, L. and G. M. Rosenblatt, Chem. Revs. 61, 257 (1961).

SILICON DIOXIDE

CONDENSED PHASE

O_2Si

Reference State for Calculating ΔH_f°, ΔF_f° and Log K_p: Solid Si from 0° to 1690°K, Liquid Si from 1690° to 3566°K, Gaseous Si from 3566° to 6000°K, Gaseous O_2; α-Quartz from 0° to 848°K, β-Quartz from 848° to 1298°K, α-Cristobalite from 1298° to 1996°K, Liquid SiO_2 from 1996° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.664	-216.820	-216.820	INFINITE
298.15	10.627	10.000	10.000	0.000	-218.000	-205.019	150.276
300	10.680	10.066	10.000	0.020	-218.002	-204.939	149.291
400	12.812	13.457	10.448	1.204	-218.036	-200.576	109.584
500	14.240	16.477	11.358	2.560	-217.960	-196.217	85.762
600	15.390	19.178	12.440	4.043	-217.807	-191.881	69.889
700	16.409	21.628	13.580	5.633	-217.585	-187.577	58.561
800	17.358	23.882	14.729	7.322	-217.299	-183.310	50.076
848	17.798	24.906	15.276	8.166	-217.139	-181.276	46.717
848	16.055	25.248	15.276	8.456	-216.849	-181.276	46.717
900	16.156	26.206	15.880	9.293	-216.759	-179.097	43.489
1000	16.350	27.919	17.000	10.919	-216.590	-174.920	38.227
1100	16.544	29.486	18.065	12.563	-216.424	-170.762	33.926
1200	16.738	30.934	19.078	14.228	-216.256	-166.618	30.344
1298	16.928	32.255	20.023	15.877	-216.092	-162.570	27.371
1298	17.048	32.394	20.023	16.057	-215.912	-162.570	27.371
1300	17.052	32.420	20.042	16.091	-215.908	-162.489	27.316
1400	17.256	33.691	20.972	17.807	-215.723	-158.387	24.724
1500	17.460	34.889	21.860	19.543	-215.[illegible]34	-154.296	22.480
1600	17.664	36.022	22.710	21.299	-215.340	-150.221	20.518
1690	17.848	36.994	23.445	22.897	-215.160	-146.564	18.953
1690	17.848	36.994	23.445	22.897	-227.110	-146.564	18.953
1700	1[illegible].868	37.099	23.525	23.075	-227.090	-146.087	18.780
1800	18.072	38.126	24.308	24.872	-226.885	-141.327	17.159
1900	18.276	39.109	25.062	26.690	-226.672	-136.581	15.710
1996	18.472	40.014	25.759	28.454	-226.460	-132.032	14.456
1996	21.660	41.067	25.759	30.554	-224.360	-132.032	14.456
2000	21.660	41.110	25.790	30.640	-224.339	-131.848	14.407
2100	21.660	42.167	26.545	32.806	-223.794	-127.238	13.241
2200	21.660	43.174	27.278	34.972	-223.255	-122.652	12.184
2300	21.660	44.137	27.990	37.138	-222.720	-118.093	11.221
2400	21.660	45.059	28.682	39.304	-222.192	-113.554	10.340
2500	21.660	45.943	29.355	41.470	-221.669	-109.040	9.532
2600	21.660	46.793	30.010	43.636	-221.151	-104.544	8.787
2700	21.660	47.610	30.646	45.802	-220.638	-100.069	8.100
2800	21.660	48.398	31.266	47.968	-220.130	-95.612	7.462
2900	21.660	49.158	31.870	50.134	-219.6[illegible]7	-91.174	6.871
3000	21.660	49.892	32.459	[illegible].300	-219.1[illegible]	-86.753	6.320
3100	21.660	50.602	33.033	54.466	-218.63[illegible]	-82.347	5.805
3200	21.660	51.290	33.593	56.632	-218.147	-77.962	5.324
3300	21.660	51.957	34.139	58.798	-217.661	-73.585	4.873
3400	21.660	52.603	34.673	60.964	-217.181	-69.226	4.450
3500	21.660	53.231	35.194	63.130	-216.704	-64.879	4.051
3565.77	21.660	53.634	35.530	64.555	-216.392	-62.026	3.801
3565.77	21.660	53.634	35.530	64.555	-307.887	-62.026	3.801
3600	21.660	53.841	35.704	65.296	-307.669	-59.672	3.622
3700	21.660	54.435	36.202	67.462	-307.035	-52.791	3.118
3800	21.660	55.012	36.689	69.628	-306.40[illegible]	-45.925	2.641
3900	21.660	55.575	37.166	71.794	-305.781	-39.080	2.190
4000	21.660	56.123	37.633	73.960	-305.158	-32.244	1.762
4100	21.660	56.658	38.091	76.126	-3[illegible]4.[illegible]41	-25.435	1.356
4200	21.660	57.180	38.539	78.292	-303.927	-18.626	0.969
4300	21.660	57.690	38.979	80.458	-303.316	-11.845	0.602
4400	21.660	58.188	39.410	92.624	-302.710	[illegible].071	0.252
4500	21.660	58.675	39.832	[illegible].790	-302.107	1.690	-0.082
4600	21.660	59.151	40.247	86.956	-301.510	8.435	-0.401
4700	21.660	59.617	40.654	89.122	-300.916	15.167	-0.705
4800	21.660	60.073	41.054	91.288	-300.329	21.885	-0.996
4900	21.660	60.519	41.447	93.454	-299.748	28.592	-1.275
5000	21.660	60.957	41.833	95.620	-299.174	35.290	-1.542
5100	21.660	61.386	42.212	97.786	-298.610	41.978	-1.799
5200	21.660	61.806	42.585	99.952	-298.055	48.651	-2.045
5300	21.660	62.219	42.951	102.118	-297.513	55.316	-2.281
5400	21.660	62.624	43.312	104.284	-296.985	61.968	-2.508
5500	21.660	63.021	43.667	106.450	-296.475	68.616	-2.726
5600	21.660	63.411	44.016	108.616	-295.987	75.250	-2.937
5700	21.660	63.795	44.359	110.782	-295.524	81.877	-3.139
5800	21.660	64.172	44.698	112.948	-295.093	88.501	-3.335
5900	21.660	64.542	45.031	115.114	-294.699	95.119	-3.523
6000	21.660	64.906	45.359	117.280	-294.349	101.728	-3.705

15 September 1963 HLS

$\Delta H^\circ_{f298.15}$ = -218.0 kcal gfw^{-1} $S^\circ_{298.15}$ = 10.00 ± 0.10 cal deg^{-1}gfw^{-1}

T_t = 848°K ΔH_t = 0.290 kcal gfw^{-1}

T_t = 1298°K ΔH_t = 0.180 kcal gfw^{-1}

T_m = 1996°K ΔH_m = 2.100 kcal gfw^{-1}

$H_{298.15} - H^\circ_0$ = 1.664 cal gfw^{-1}

$C^\circ_p = 11.22 + 8.20 \times 10^{-3}T - 2.70 \times 10^5 T^{-2}$ cal deg K^{-1} gfw^{-1} 298.15°K ≤ T ≤ 848°K

$C^\circ_p = 14.41 + 1.94 \times 10^{-3}T$ cal degK^{-1} gfw^{-1} 848°K ≤ T ≤ 1298°

$C^\circ_p = 14.40 + 2.04 \times 10^{-3}T$ cal degK^{-1}gfw^{-1} 1298°K ≤ T ≤ 1996°K

C°_p = 21.66 degK^{-1}gfw^{-1} 1996°K ≤ T ≤ 6000°K

Structure

The stable forms of SiO_2 are considered to be: α-quartz (hexagonal) up to 848°K; β-quartz (hexagonal) up to 1298°K, β-cristobalite (cubic) up to 1996°K

Heat of Formation

Average of calorimetric values by Golutvin[1], Wise, et al[2], Good, et al [3]

Heat Capacity and Entropy

Low-temperature data from Anderson[4] and Kelley and King [5] High-temperature data from Kelley.[6] Data above melting point from Schick. [7]

Melting and Vaporization

Heat of fusion was an average value from Schick. [7]

References

1. Golutvin, Yu, Zh. Fiz. Khim. 30, 2251 (1956)
2. Wises, et al, S. S. J. Phys. Chem. 67, 815 (1963).
3. Good, W., et al, J. Phys. Chem. 66, 380 (1962)
4. Anderson, C. T., J. Am. Chem. Soc. 58, 568 (1936)
5. Kelley, K. K., King, E. G., Bur. Mines Bull. 592 (1961).
6. Kelley, K. K., Bur. of Mines Bull., 584 (1960).
7. Schick, H., Chem. Revs. 60, (1963).

SILICON DIOXIDE (SiO_2) (CONDENSED PHASE) GFW = 60.09

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/K gfw)	S°_T (cal/K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal/gfw)	ΔH_f (Kcal/gfw)	ΔF_f (Kcal/gfw)	Log K_p
298.15	±0.100	±0.100	±0.100	±0.000	±0.500		
848	±0.100	±0.205	±0.140	±0.055			
848	±0.200	±0.240	±0.140	±0.085			
1000	±0.200	±0.273	±0.157	±0.115			
1298	±0.200	±0.325	±0.190	±0.175			
1298	±0.200	±0.364	±0.190	±0.225			
1996	±0.200	±0.450	±0.267	±0.365			
1996	±1.000	±0.951	±0.267	±1.365			
2000	±1.000	±0.953	±0.268	±1.369			
3000	±1.000	±1.358	±0.569	±2.369			
4000	±1.000	±1.646	±0.804	±3.369			
5000	±1.000	±1.869	±0.995	±4.369			
6000	±1.000	±2.051	±1.156	±5.369			

<u>TABLE 200</u>

SILICON DIOXIDE

IDEAL MOLECULAR GAS

O_2Si

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Si from 0° to 1690°K, Liquid Si from 1690° to 3566°K, Gaseous Si from 3566° to 6000°K, Gaseous O_2; Gaseous SiO_2.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.517	-77.106	-77.106	INFINITE
298.15	10.467	54.526	54.526	0.000	-77.433	-77.728	56.973
300	10.486	54.590	54.526	0.019	-77.436	-77.730	56.623
400	11.425	57.741	54.949	1.117	-77.556	-77.809	42.511
500	12.162	60.373	55.778	2.298	-77.655	-77.860	34.031
600	12.727	62.643	56.737	3.543	-77.740	-77.893	28.371
700	13.154	64.638	57.726	4.838	-77.813	-77.912	24.324
800	13.477	66.417	58.703	6.171	-77.883	-77.923	21.286
900	13.724	68.019	59.651	7.531	-77.954	-77.923	18.922
1000	13.916	69.475	60.561	8.914	-78.028	-77.914	17.027
1100	14.066	70.809	61.433	10.313	-78.107	-77.899	15.476
1200	14.186	72.038	62.266	11.726	-78.191	-77.877	14.183
1300	14.283	73.178	63.063	13.150	-78.282	-77.849	13.087
1400	14.362	74.239	63.823	14.582	-78.381	-77.811	12.146
1500	14.427	75.232	64.551	16.022	-78.488	-77.766	11.330
1600	14.481	76.165	65.248	17.467	-7[illegible].605	-77.715	10.615
1690	14.523	76.959	65.851	18.772	-78.718	-77.663	10.043
1690	14.523	76.959	65.851	18.772	-90.668	-77.663	10.043
1700	14.527	77.044	65.917	18.917	-90.681	-77.586	9.974
1800	14.566	77.876	66.558	20.372	-90.818	-76.810	9.326
1900	14.599	78.664	67.175	21.830	-90.965	-76.029	8.745
2000	14.627	79.414	67.768	23.292	-91.120	-75.237	8.221
2100	14.652	80.128	68.340	24.756	-91.277	-74.440	7.747
2200	14.674	80.810	68.891	26.222	-91.438	-73.634	7.314
2300	14.693	61.463	69.424	27.690	-91.601	-72.824	6.920
2400	14.710	82.084	69.938	29.161	-91.768	-72.002	6.556
2500	14.725	82.689	70.437	30.632	-91.940	-71.178	6.222
2600	14.738	83.267	70.919	32.105	-92.115	-70.340	5.912
2700	14.750	83.824	71.387	33.580	-92.293	-69.503	5.626
2800	14.760	84.360	71.841	35.055	-92.476	-68.655	5.359
2900	14.770	84.878	72.281	36.532	-92.662	-67.799	5.109
3000	14.778	85.379	72.710	38.009	-92.853	-66.939	4.876
3100	14.786	85.864	73.126	39.487	-93.047	-66.068	4.658
3200	14.793	86.334	73.532	40.966	-93.246	-65.199	4.453
3300	14.800	86.789	73.926	42.446	-9[illegible].446	-64.315	4.259
3400	14.806	87.231	74.311	43.926	-93.[illegible]2	-63.428	4.077
3500	14.811	87.660	74.687	45.407	-93.[illegible]	-62.537	3.905
3565.77	14.815	87.936	74.928	46.382	-93.998	-61.943	3.796
3565.77	14.815	87.936	74.928	46.382	-185.493	-61.943	3.796
3600	14.816	88.077	75.053	46.889	-185.509	-60.761	3.689
3700	14.821	88.483	75.410	48.371	-185.559	-57.294	3.384
3800	14.825	88.879	75.760	49.853	-185.614	-53.827	3.096
3900	14.829	89.264	76.101	51.336	-185.672	-50.359	2.822
4000	14.833	89.639	76.435	52.819	-185.732	-46.885	2.562
4100	14.836	90.006	76.761	54.302	-185.798	-43.415	2.314
4200	14.840	90.363	77.081	55.786	-185.866	-39.935	2.078
4300	14.843	90.712	77.394	57.270	-185.937	-36.463	1.853
4400	14.845	91.054	77.700	58.755	-186.012	-32.980	1.638
4500	14.848	91.387	78.001	60.239	-186.091	-29.503	1.433
4600	14.850	91.714	78.295	61.724	-186.175	-26.019	1.236
4700	14.853	92.033	78.584	63.209	-186.262	-22.537	1.048
4800	14.855	92.346	78.868	64.695	-186.355	-19.055	0.868
4900	14.857	92.652	79.146	66.180	-186.455	-15.566	0.694
5000	14.859	92.952	79.419	67.666	-186.561	-12.073	0.528
5100	14.860	93.247	79.687	69.152	-186.677	-8.578	0.368
5200	14.862	93.535	79.951	70.638	-186.802	-5.085	0.214
5300	14.864	93.818	80.210	72.124	-186.940	-1.590	0.066
5400	14.865	94.096	80.464	73.611	-187.091	1.915	-0.077
5500	14.866	94.369	80.715	75.097	-187.261	5.419	-0.215
5600	14.868	94.637	80.961	76.584	-187.452	8.925	-0.348
5700	14.869	94.900	81.203	78.071	-187.668	12.433	-0.477
5800	14.870	95.159	81.442	79.558	-187.916	15.953	-0.601
5900	14.871	95.413	81.676	81.045	-188.201	19.480	-0.722
6000	14.873	95.663	81.907	82.532	-188.530	23.007	-0.838

15 September 1963 HLS

SILICON DIOXIDE (SiO_2) (IDEAL MOLECULAR GAS) gfw = 60.09

ΔH°_{f0} = -77.106 kcal gfw^{-1}

$\Delta H^\circ_{f298.15}$ = -77.433 kcal gfw^{-1}

Point Group $D_{\infty h}$

$S^\circ_{298.15}$ = 54.526 cal deg^{-1} gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 2.517 kcal gfw^{-1}

Vibrational Levels and Multiplicities

ω, cm^{-1}	ω, cm^{-1}
990.9 (1)	1449.3 (1)
377.9 (2)	

Bond lengths and angles:

Si-O distance = 1.509 A

O-Si-O angle = 180°

Moment of inertia:

I = 12.0976 x 10^{-39} gm cm^2

B_e = 0.23135 cm^{-1}

Heat of Formation

Vapor-pressure data of Porter et al[1] was used. Results in general agreement with earlier analyses by Schick[2] and Brewer and Rosenblatt.[3]

Heat Capacity and Entropy

Estimated values for spectroscopic constants were used.

References

1. Porter, R., et al, J. Chem. Phys. 23, 216 (1955).
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SILICON DIOXIDE (SiO_2) (IDEAL MOLECULAR GAS) GFW = 60.09

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal/gfw)	ΔH_f (Kcal/gfw)	ΔF_f (Kcal/gfw)	Log K_p
298.15	±1.000	±1.000	±1.000	±0.000	±5.000		
1000	±1.000	±2.210	±1.508	±0.702			
2000	±1.000	±2.903	±2.052	±1.702			
3000	±1.000	±3.309	±2.408	±2.702			
4000	±1.000	±3.596	±2.671	±3.702			
5000	±1.000	±3.820	±2.879	±4.702			
6000	±1.000	±4.002	±3.052	±5.702			

TABLE 201

TANTALUM DIOXIDE — **IDEAL MOLECULAR GAS** — **O_2Ta**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ta from 0° to 3270°K, Liquid Ta from 3270° to 5706°K, Gaseous Ta from 5706° to 6000°K; Gaseous O_2; Gaseous TaO_2.

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-2.675	-45.950	-45.950	INFINITE
298.15	11.071	62.527	62.527	0.000	-46.708	-47.781	35.023
300	11.091	62.595	62.527	0.020	-46.712	-47.788	34.812
400	12.022	65.919	62.974	1.178	-46.883	-48.120	26.290
500	12.725	68.681	63.847	2.417	-47.008	-48.413	21.161
600	13.231	71.048	64.854	3.716	-47.107	-48.684	17.732
700	13.594	73.117	65.890	5.059	-47.190	-48.941	15.279
800	13.862	74.950	66.910	6.432	-47.271	-49.186	13.436
900	14.068	76.595	67.897	7.829	-47.348	-49.421	12.000
1000	14.235	78.086	68.842	9.244	-47.427	-49.646	10.850
1100	14.380	79.450	69.745	10.675	-47.504	-49.864	9.907
1200	14.513	80.707	70.607	12.120	-47.582	-50.075	9.120
1300	14.639	81.874	71.430	13.578	-47.660	-50.282	8.453
1400	14.761	82.963	72.215	15.048	-47.739	-50.480	7.880
1500	14.881	83.986	72.966	16.530	-47.820	-50.672	7.383
1600	14.999	84.950	73.685	18.024	-47.902	-50.860	6.947
1700	15.113	85.863	74.375	19.529	-47.[illegible]96	-51.043	6.562
1800	15.223	86.730	75.037	21.046	-48.073	-51.219	6.219
1900	15.328	87.555	75.675	22.574	-48.162	-51.393	5.911
2000	15.426	88.344	76.288	24.112	-48.259	-51.558	5.634
2100	15.518	89.099	76.881	25.659	-48.364	-51.723	5.383
2200	15.602	89.823	77.453	27.215	-48.477	-51.878	5.153
2300	15.678	90.518	78.006	28.779	-48.603	-52.030	4.944
2400	15.746	91.187	78.541	30.350	-48.744	-52.178	4.751
2500	15.806	91.831	79.060	31.928	-48.908	-52.318	4.573
2600	15.859	92.452	79.563	33.511	-49.090	-52.449	4.409
2700	15.904	93.051	80.052	35.099	-49.307	-52.575	4.255
2800	15.942	93.630	80.526	36.692	-49.563	-52.692	4.113
2900	15.974	94.190	80.988	36.288	-49.873	-52.798	3.979
3000	16.000	94.732	81.437	39.886	-50.247	-52.894	3.853
3100	16.019	95.257	81.874	41.487	-50.692	-52.970	3.734
3200	16.034	95.766	82.301	43.090	-51.217	-53.041	3.622
3270	16.042	96.113	82.593	44.213	-51.634	-53.075	3.547
3270	16.042	96.113	82.593	44.213	-58.334	-53.075	3.547
3300	16.044	96.260	82.716	44.694	-58.398	-53.024	3.511
3400	16.050	96.739	83.122	46.299	-58.61[illegible]	-52.862	3.398
3500	16.052	97.204	83.517	4[illegible].704	-58.83[illegible]	-52.682	3.289
3600	16.051	97.656	83.904	49.509	-59.055	-52.508	3.187
3700	16.047	98.096	84.281	51.114	-59.281	-52.321	3.090
3800	16.041	98.524	84.651	52.718	-59.512	-52.131	2.998
3900	16.032	98.940	85.012	54.322	-59.[illegible]47	-51.934	2.910
4000	16.021	99.346	85.365	55.925	-59.986	-51.728	2.826
4100	16.009	99.742	85.711	57.526	-60.231	-51.521	2.746
4200	15.995	100.127	86.050	59.126	-60.481	-51.303	2.669
4300	15.980	100.503	86.381	60.725	-60.735	-51.077	2.596
4400	15.964	100.871	86.707	62.322	-60.996	-50.853	2.526
4500	15.948	101.229	87.025	63.918	-61.261	-50.618	2.458
4600	15.931	101.580	87.338	65.512	-61.533	-50.374	2.393
4700	15.913	101.922	87.645	67.104	-61.812	-50.130	2.331
4800	15.895	102.257	87.945	68.695	-62.098	-49.871	2.271
4900	15.877	102.584	88.241	70.283	-62.393	-49.619	2.213
5000	15.858	102.905	88.531	71.870	-62.697	-49.353	2.157
5100	15.840	103.219	88.816	[illegible].455	-63.012	-49.080	2.103
5200	15.821	103.526	89.096	75.036	-63.339	-48.804	2.051
5300	15.803	103.827	89.371	76.619	-63.681	-48.521	2.001
5400	15.784	104.123	89.641	78.198	-64.040	-48.225	1.952
5500	15.766	104.412	89.907	79.776	-64.417	-47.923	1.904
5600	15.748	104.696	90.169	81.352	-64.818	-47.621	1.858
5700	15.731	104.975	90.426	82.926	-65.246	-47.306	1.814
5706.65	15.729	104.993	90.443	83.030	-65.276	-47.284	1.811
5706.65	15.729	104.993	90.443	83.030	-246.499	-47.284	1.811
5800	15.713	105.248	90.679	84.498	-247.084	-44.017	1.659
5900	15.696	105.516	90.929	86.068	-247.753	-40.513	1.501
6000	15.679	105.780	91.174	87.637	-248.470	-36.982	1.347

15 September 1963 HLS

TANTALUM DIOXIDE (TaO_2) (IDEAL MOLECULAR GAS) gfw = 212.95

ΔH°_{f0} = -45.950 kcal. gfw^{-1}

$\Delta H^{\circ}_{f298.15}$ = -46.708 kcal gfw^{-1}

Point Group $D_{\infty h}$

$S^{\circ}_{298.15}$ = 62.527 cal deg K^{-1} gfw^{-1}

$H^{\circ}_{298.15} - H^{\circ}_{0}$ = 2.675 kcal gfw^{-1}

Vibrational Levels and Multiplicities

ω, cm^{-1}	ω, cm^{-1}
988.9 (1)	1072.8 (1)
279.7 (2)	

Bond lengths and angles:

Ta - O distance = 1.687 A

O-Ta-O angle = 180°

Moments of inertia

$I = 15.12 \times 10^{-39}$ gm cm^2 $\sigma = 2$

$B_e = 0.185111$ cm^{-1}

Heat of Formation

Vaporization data of Inghram et al[1] was used.

Heat Capacity and Entropy

Spectroscopic constants were estimated. See volume 1, this study (section IVB27.4.2) for details.

Reference

1. Inghram, M., W. Chupka, and J. Berkowitz, J. Chem. Phys. 27, 569 (1957)

TANTALUM DIOXIDE (TaO_2) (IDEAL MOLECULAR GAS) GFW = 212.95

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^{\circ} - H_{298}^{\circ})/T$ (cal/°K gfw)	$H_T^{\circ} - H_{298}^{\circ}$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
298.15	±1.000	±3.000	±3.000	±0.000	±10.000		
1000	±1.000	±4.210	±3.508	±0.702			
2000	±1.000	±4.903	±4.052	±1.702			
3000	±1.000	±5.309	±4.408	±2.702			
4000	±1.000	±5.596	±4.671	±3.702			
5000	±1.000	±5.820	±4.879	±4.702			
6000	±1.000	±6.002	±5.052	±5.702			

TABLE 202

TITANIUM DIOXIDE CONDENSED PHASE O_2Ti

Reference State for Calculating ΔH_f°, ΔF_f°, and Log Kp: Solid Ti from 0° to 1950°K, Liquid Ti from 1950° to 3550°K, Gaseous Ti from 3550° to 6000°K; Gaseous O_2; Solid TiO_2 from 0° to 2143°K, Liquid TiO_2 from 2143° to 6000°K.

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-2.064	-224.639	-224.639	INFINITE
298.15	13.160	12.040	12.040	0.000	-225.800	-212.593	155.827
300	13.221	12.122	12.040	0.024	-225.800	-212.511	154.807
400	15.363	16.262	12.590	1.469	-225.685	-208.094	113.692
500	16.370	19.810	13.689	3.061	-225.473	-203.720	89.042
600	16.930	22.849	14.969	4.728	-225.235	-199.392	72.625
700	17.278	25.487	16.287	6.440	-224.994	-195.104	60.911
800	17.514	27.810	17.585	8.180	-224.762	-190.850	52.135
900	17.685	29.884	18.838	9.941	-224.540	-186.623	45.316
1000	17.815	31.754	20.038	11.716	-224.333	-182.421	39.866
1100	17.918	33.457	21.182	13.503	-224.139	-178.240	35.411
1155	17.967	34.332	21.787	14.490	-224.037	-175.947	33.291
1155	17.967	34.332	21.787	14.490	-224.987	-175.947	33.291
1200	18.004	35.020	22.271	15.299	-224.907	-174.038	31.695
1300	18.077	36.464	23.308	17.103	-22[illegible].738	-169.808	28.546
1400	18.140	37.806	24.296	18.914	-224.581	-165.587	25.848
1500	18.197	39.059	25.239	20.731	-224.434	-161.379	23.512
1600	18.248	40.235	26.140	22.553	-224.300	-157.181	21.469
1700	18.295	41.343	27.002	24.380	-224.177	-152.989	19.667
1800	18.340	42.390	27.828	26.212	-224.065	-148.805	18.067
1900	18.382	43.383	28.620	28.048	-223.964	-144.624	16.635
1950	18.402	43.860	29.005	28.968	-223.917	-142.537	15.974
1950	18.402	43.860	29.005	28.968	-227.617	-142.537	15.974
2000	18.421	44.327	29.382	29.888	-227.549	-140.356	15.337
2100	18.459	45.226	30.116	31.732	-227.411	-136.002	14.153
2143	18.475	45.601	30.423	32.526	-227.352	-134.131	13.678
2143	18.475	52.600	30.423	47.526	-212.352	-134.131	13.678
2200	18.475	53.085	31.003	48.580	-212.274	-132.049	13.117
2300	18.475	53.906	31.982	50.427	-212.143	-128.409	12.201
2400	18.475	54.693	32.912	52.275	-212.017	-124.770	11.361
2500	18.475	55.447	33.798	54.122	-211.898	-121.138	10.589
2600	18.475	56.171	34.645	55.970	-211.782	-117.507	9.877
2700	18.475	56.869	35.455	57.817	-211.673	-113.885	9.218
2800	18.475	57.541	36.232	59.665	-211.567	-110.264	8.606
2900	18.475	58.189	36.978	61.512	[illegible]	-106.648	8.037
3000	18.475	58.815	37.695	63.360	-211.[illegible]	-103.034	7.506
3100	18.475	59.421	38.386	65.207	-211.282	-99.422	7.009
3200	18.475	60.008	39.053	67.055	-211.196	-95.819	6.544
3300	18.475	60.576	39.697	68.902	-211.114	-92.213	6.107
3400	18.475	61.128	40.319	70.750	-211.036	-88.610	5.696
3500	18.475	61.663	40.921	72.597	-210.963	-85.009	5.308
3550	18.475	61.925	41.215	73.521	-210.927	-83.211	5.122
3550	18.475	61.925	41.215	73.521	-313.384	-83.211	5.122
3600	18.475	62.184	41.505	74.445	-313.355	-79.971	4.855
3700	18.475	62.690	42.070	76.292	-313.309	-73.486	4.340
3800	18.475	63.182	42.619	78.140	-313.280	-67.002	3.853
3900	18.475	63.662	43.153	79.987	-313.270	-60.526	3.392
4000	18.475	64.130	43.671	81.835	-313.274	-54.040	2.952
4100	18.475	64.586	44.176	83.682	-313.296	-47.561	2.535
4200	18.475	65.032	44.667	85.530	-313.333	41.076	2.137
4300	18.475	65.466	45.146	87.377	-313.386	-44.592	1.758
4400	18.475	65.891	45.613	89.225	-313.454	-28.108	1.396
4500	18.475	66.306	46.068	91.072	-313.537	-21.626	1.050
4600	18.475	66.712	46.512	92.920	-313.634	-15.129	0.719
4700	18.475	67.110	46.946	94.767	-313.748	-8.641	0.402
4800	18.475	67.499	47.370	96.615	-313.876	-2.144	0.098
4900	18.475	67.879	47.785	98.462	-314.020	4.353	-0.194
5000	18.475	68.253	48.191	100.310	-314.179	10.850	-0.474
5100	18.475	68.619	48.588	102.157	-314.357	17.353	-0.744
5200	18.475	68.977	48.976	104.005	-314.551	23.862	-1.003
5300	18.475	69.329	49.357	105.852	-314.766	30.375	-1.252
5400	18.475	69.675	49.730	107.700	-315.002	36.888	-1.493
5500	18.475	70.014	50.096	109.547	-315.262	43.414	-1.725
5600	18.475	70.346	50.455	111.395	-315.549	49.933	-1.949
5700	18.475	70.673	50.806	113.242	-315.867	56.475	-2.165
5800	18.475	70.995	51.152	115.090	-316.221	63.011	-2.374
5900	18.475	71.311	51.491	116.937	-316.617	69.560	-2.577
6000	18.475	71.621	51.824	118.785	-317.060	76.114	-2.772

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TITANIUM DIOXIDE (TiO_2) (CONDENSED PHASE) gfw = 79.90

$\Delta H^\circ_{f298.15}$ = -225.8 kcal gfw^{-1} $S^\circ_{298.15}$ = 12.04 cal deg^{-1} gfw^{-1}

T_m = 2143 °K ΔH_m = 15.0 kcal gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 2.064 kcal gfw^{-1}

$C^\circ_p = 17.97 + 0.28 \times 10^{-3}T - 4.35 \times 10^5 T^{-2}$ cal deg^{-1} gfw^{-1} 298.15 °K ≤ T ≤ 2143 °K

C°_p = 18.475 cal deg K^{-1} gfw^{-1} 2143 °K ≤ T ≤ 6000 °K

The stable form of TiO_2 is rutile with a tetragonal structure.

Heat of Formation

Based on combustion data of Mah *et al*[1] and agreeing with Humphrey,[2] and Ariya *et al*[3].

Heat Capacity and Entropy

Low-temperature data based on Kelley and King analysis.[4] High-temperature data from Kelley.[5] Data above melting point is estimated.

Melting and Vaporization

Melting point is from Brauer and Littke.[6] Heat of fusion was estimated.

References

1. Mah, A. *et al*, Bur. of Mines Rept. 5316 (1957).
2. Humphrey, G. L., J. Am. Chem. Soc. 73, 1587 (1951).
3. Ariya, S., *et al*, J. Inorg. Chem. (Russia) 3, 13 (1957).
4. Kelley, K., E. G. King., Bur. of Mines Bull. 592 (1961).
5. Kelley, K., Bur. of Mines Bull. 584 (1960).
6. Brauer, G., W. J. Littke., J. Inorg. Nucl. Chem. 16, 67 (1960).

TITANIUM DIOXIDE (TiO_2) (CONDENSED PHASE) GFW = 79.90

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal/gfw)	ΔH°_f (Kcal/gfw)	ΔF°_f (Kcal/gfw)	Log K_p
298.15	±0.200	±0.040	±0.040	±0.000	±1 000		
1000	±0.200	±0.282	±0.142	±0.140			
2000	±0.200	±0.421	±0.250	±0.340			
2143	±0.200	±0.434	±0.262	±0.369			
2143	±2.000	±2.768	±0.262	±5.369			
3000	±2.000	±3.440	±1.079	±7.083			
4000	±2.000	±4.016	±1.745	±9.083			
5000	±2.000	±4.462	±2.246	±11.083			
6000	±2.000	±4.827	±2.646	±13.083			

TITANIUM DIOXIDE — IDEAL MOLECULAR GAS — O_2Ti

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ti from 0° to 1950°K, Liquid Ti from 1950° to 3550°K, Gaseous Ti from 3550° to 6000°K; Gaseous O_2, Gaseous TiO_2.

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-2.662	-82.327	-82.327	INFINITE
298.15	11.120	56.562	56.562	0.000	-82.890	-82.957	60.806
300	11.140	56.631	56.562	0.021	-82.893	-82.957	60.432
400	12.091	59.972	57.011	1.184	-83.060	-82.953	45.321
500	12.788	62.749	57.889	2.430	-83.194	-82.910	36.238
600	13.283	65.127	58.902	3.735	-83.318	-82.841	30.174
700	13.635	67.203	59.942	5.082	-83.442	-82.752	25.835
800	13.889	69.041	60.967	6.459	-83.573	-82.645	22.577
900	14.078	70.688	61.957	7.858	-83.713	-82.520	20.038
1000	14.220	72.179	62.906	9.273	-83.866	-82.379	18.003
1100	14.329	73.540	63.812	10.701	-84.031	-82.223	16.335
1155	14.378	74.240	64.292	11.490	-84.127	-82.130	15.540
1155	14.378	74.240	64.292	11.490	-85.077	-82.130	15.540
1200	14.415	74.790	64.675	12.138	-85.158	-82.013	14.936
1300	14.483	75.947	65.498	13.583	-85.348	-81.745	13.742
1400	14.538	77.022	66.284	15.034	-85.551	-81.461	12.716
1500	14.583	78.027	67.033	16.490	-85 765	-81.160	11.825
1600	14.620	78.969	67.750	17.950	-85.993	-80.847	11.043
1700	14.652	79.856	68.436	19.414	-86.233	-80.517	10.351
1800	14.678	80.695	69.094	20.881	-86.486	-80.174	9.734
1900	14.701	81.489	69.726	22.349	-86.753	-79.816	9.180
1950	14.711	81.871	70.033	23.085	-86.890	-79.632	8.924
1950	14.711	81.871	70.033	23.085	-90.590	-79.632	8.924
2000	14.720	82.243	70.333	23.821	-90.706	-79.348	8.670
2100	14.737	82.962	70.918	25.293	-90.940	-78.776	8.198
2200	14.751	83.648	71.481	26.768	-91.176	-78.191	7.767
2300	14.764	84.304	72.024	28.244	-91.416	-77.595	7.373
2400	14.775	84.933	72.549	29.721	-91.661	-76.988	7.010
2500	14.785	85.536	73.056	31.199	-91.911	-76.372	6.676
2600	14.794	86.116	73.548	32.678	-92.164	-75.745	6.367
2700	14.802	86.674	74.024	34.157	-92.423	-75.111	6.080
2800	14.809	87.213	74.485	35.638	-92.694	-74.462	5.812
2900	14.816	87.733	74.933	37.119	-92.951	-73.807	5.562
3000	14.821	88.235	75.368	38.601	-93.221	-73.143	5.328
3100	14.827	88.721	75.791	40.084	-93.495	-72.468	5.109
3200	14.831	89.192	76.202	41.566	-93.77[illegible]	-71.786	4.903
3300	14.836	89.648	76.603	43.050	-94.05[illegible]	-71.092	4.708
3400	14.840	90.091	76.993	44.534	-94.34	-70.392	4.525
3500	14.843	90.522	77.374	46.018	-94.632	-69.684	4.351
3550	14.845	90.732	77.560	46.760	-94.778	-69.325	4.268
3550	14.845	90.732	77.560	46.760	-197.235	-69.325	4.268
3600	14.847	90.940	77.745	47.502	-197.388	-67.525	4.099
3700	14.850	91.347	78.107	48.987	-197.704	-63.913	3.775
3800	14.852	91.743	78.460	50.472	-198.038	-60.288	3.467
3900	14.855	92.128	78.806	51.957	-198.390	-56.662	3.175
4000	14.857	92.505	79.144	53.443	-198.756	-53.022	2.897
4100	14.860	92.871	79.474	54.929	-199.139	-49.373	2.632
4200	14.862	93.230	79.797	56.415	-199.538	-45.712	2.379
4300	14.864	93.579	80.114	57.901	-199.952	-42.044	2.137
4400	14.866	93.921	80.424	59.388	-200.381	-38.366	1.906
4500	14.867	94.255	80.727	60.874	-200.825	-34.681	1.684
4600	14.869	94.582	81.025	62.361	-201.283	-30.979	1.472
4700	14.870	94.902	81.317	3.848	-201.757	-27.275	1.268
4800	14.872	95.215	81.603	65.335	-202.246	-23.552	1.072
4900	14.873	95.521	81.884	66.823	-202.749	-19.822	0.884
5000	14.874	95.822	82.160	68.310	-203.269	-16.085	0.703
5100	14.875	96.117	82.431	69.797	-203.807	-12.337	0.529
5200	14.877	96.405	82.697	71.285	-204.361	-8.577	0.360
5300	14.878	96.689	82.958	72.773	-204.935	-4.800	0.198
5400	14.879	96.967	83.215	74.261	-205.531	-1.021	0.041
5500	14.880	97.240	83.467	75.748	-206.151	2.784	-0.111
5600	14.880	97.508	83.716	77.236	-206.798	6.581	-0.257
5700	14.881	97.771	83.960	78.724	-207.475	10.408	-0.399
5800	14.882	98.030	84.200	80.213	-208.188	14.243	-0.537
5900	14.883	98.265	84.437	81.701	-208.943	18.088	-0.670
6000	14.883	98.535	84.670	83.189	-209.746	21.948	-0.799

15 September 1963 — HLS

TITANIUM DIOXIDE (TiO_2) (IDEAL MOLECULAR GAS) gfw = 79.90

ΔH°_{f0} = -82.327 kcal gfw^{-1}

$\Delta H^\circ_{f298.15}$ = -82.890 kcal gfw^{-1}

Point Group $D_{\infty h}$

$S^\circ_{298.15}$ = 56.562 cal deg K^{-1} gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 2.662 kcal gfw^{-1}

Vibrational Levels and Multiplicities

ω, cm^{-1}	ω, cm^{-1}
873.2 (1)	1127.8 (1)
294.1 (2)	

Bond lengths and angles:

O-Ti distance = 1.620 Å

O-Ti-O angle = 180°

Moments of inertia:

$I = 13.9429 \times 10^{-39}$ gcm^2 $\sigma = 2$

$B_e = 0.20074$ cm^{-1}

Heat of Formation

Vaporization data of Berkowitz et al[1] was recalculated.

Heat Capacity and Entropy

Estimated spectroscopic constants were used.

Reference

1. Berkowitz, J., et al, J. Phys. Chem. 61 1569 (1957)

TITANIUM DIOXIDE (TiO_2) (IDEAL MOLECULAR GAS) GFW = 79.90

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal/gfw)	ΔH°_f (Kcal/gfw)	ΔF°_f (Kcal/gfw)	Log K_p
298.15	±1.000	±3.000	±3.000	±0.000	±5.000		
1000	±1.000	±4.210	±3.508	±0.702			
2000	±1.000	±4.903	±4.052	±1.702			
3000	±1.000	±5.309	±4.408	±2.702			
4000	±1.000	±5.596	±4.671	±3.702			
5000	±1.000	±5.820	±4.879	±4.702			
6000	±1.000	±6.002	±5.052	±5.702			

URANIUM DIOXIDE

CONDENSED PHASE

O_2U

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid U from 0° to 1406°K, Liquid U from 1406° to 4124°K, Gaseous U from 4124° to 6000°K, Gaseous O_2; Solid UO_2 from 0° to 3000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.726	-258.550	-258.550	INFINITE
298.15	15.350	18.629	18.629	0.000	-259.200	-246.500	188.729
300	15.360	18.724	18.631	0.028	-259.197	-246.469	179.530
400	17.373	23.445	19.263	1.074	-258.940	-242.200	132.373
500	18.426	27.446	20.508	3.469	-258.613	-238.159	104.094
600	19.072	30.667	21.956	5.346	-258.279	-234.100	85.267
700	19.526	33.642	23.440	7.277	-257.982	-230.094	71.855
800	19.877	36.474	24.913	9.248	-257.755	-226.127	61.772
900	20.169	38.852	26.331	11.251	-257.617	-222.182	53.951
940	20.275	39.711	26.882	12.060	-257.595	-220.608	51.289
940	20.275	39.711	26.882	12.060	-258.278	-220.608	51.289
1000	20.424	40.971	27.890	13.281	-258.104	-218.207	47.687
1048	20.537	41.931	28.320	14.264	-258.069	-216.291	45.105
1048	20.537	41.931	28.320	14.264	-259.189	-216.291	45.105
1100	20.655	42.926	28.967	15.335	-259.032	-214.160	42.549
1200	20.869	44.735	30.223	17.411	-258.719	-210.101	38.265
1300	21.072	46.413	31.407	19.508	-258.394	-206.064	34.041
1400	21.266	47.962	32.535	21.625	-258.056	-202.051	31.540
1406	21.277	48.073	32.601	21.755	-258.035	-201.812	31.300
1406	21.277	48.073	32.601	21.755	-262.735	-201.812	31.300
1500	21.454	49.455	33.615	23.761	-262.405	-197.749	28.811
1600	21.637	50.846	34.647	25.916	-262.042	-193.451	26.425
1700	21.817	52.163	35.640	28.088	-261.667	-189.174	24.317
1800	21.994	53.415	36.595	30.279	-261.281	-184.922	22.432
1900	22.168	54.609	37.510	32.487	-260.882	-180.691	20.785
2000	22.341	55.750	38.394	34.713	-260.471	-176.476	19.264
2100	22.512	56.845	39.247	36.955	-260.055	-172.291	17.930
2200	22.682	57.896	40.071	39.215	-259.616	-168.120	16.700
2300	22.851	58.908	40.868	41.492	-259.170	-163.973	15.580
2400	23.019	59.884	41.640	43.785	-258.714	-159.843	14.555
2500	23.187	60.827	42.389	46.096	-258.246	-155.734	13.614
2600	23.353	61.740	43.116	48.425	-257.766	-151.642	12.740
2700	23.520	62.624	43.822	50.760	-257.270	-147.571	11.944
2800	23.685	63.482	44.509	53.126	-256.773	-143.514	11.201
2900	23.851	64.317	45.177	55.503	-256.257	-139.481	10.511
3000	24.016	65.128	45.827	57.891	[illegible]	-135.462	9.868

15 June 1963 MBP

URANIUM DIOXIDE (UO_2) (CONDENSED PHASE) gfw = 270.07

$\Delta H^{\circ}_{f298.15} = -259.2 \pm 0.6$ kcal gfw^{-1} $S^{\circ}_{298.15} = 18.63$ cal deg K^{-1} gfw^{-1}

T_m = Uncertain. See volume 1, this study (section IVB32.4.2).

$H^{\circ}_{298.15} - H^{\circ}_0 = 2.726$ kcal gfw^{-1}

C°_p data have been selected and smoothed (see below).

Structure

Face-centered-cubic CaF_4-type.

Heat of Formation

Taken from Coughlin.[1]

Heat Capacity and Entropy

Low-temperature data are from Jones, Gordon, and Long[2] joined to Kelley's equation.[3]

Melting and Vaporization

See volume 1, this study (section IVB32.4.2).

References

1. Coughlin, V. P., U.S. Bur. Mines, Bull. 542 (1954).
2. Jones, W. M., J. Gordon, and E. A. Long, J. Chem. Phys. 20, 695 (1952).
3. Kelley, K. K., U.S. Bur. Mines, Bull. 584 (1960).

URANIUM DIOXIDE (UO_2) (CONDENSED PHASE) GFW = 270.07

SUMMARY OF UNCERTAINTY ESTIMATES

T °K	cal/°K gfw			Kcal/gfw			
	C°_p	S°_T	$-(F^{\circ}_T - H^{\circ}_{298})/T$	$H^{\circ}_T - H^{\circ}_{298}$	ΔH_f	ΔF_f	Log K_p
298.15	± 0.200	± 0.100	± 0.100	± 0.000	± 0.600		
500	± 0.200	± 0.203	± 0.123	± 0.040			
500	± 0.500	± 0.203	± 0.123	± 0.040			
1000	± 0.500	± 0.550	± 0.260	± 0.290			
2000	± 0.500	± 0.897	± 0.501	± 0.790			
2000	± 1.000	± 0.897	± 0.501	± 0.790			
3000	± 1.000	± 1.302	± 0.705	± 1.790			

TABLE 205

URANIUM DIOXIDE | **IDEAL MOLECULAR GAS** | O_2U

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p. Solid U from 0° to 1406°K, Liquid U from 1406° to 4124°K, Gaseous U from 4124° to 6000°K; Gaseous O_2, Gaseous UO_2

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.629	-116.033	-116.033	INFINITE
298.15	10.386	68.200	68.200	0.000	-117.000	-119.146	87.332
300	10.406	68.265	68.201	0.019	-117.006	-119.160	86.804
400	11.362	71.396	68.621	1.110	-117.310	-119.831	65.469
500	12.036	74.009	69.445	2.282	-117.600	-120.427	52.636
600	12.497	76.247	70.396	3.510	-117.915	-120.964	44.059
700	12.817	78.198	71.374	4.777	-118.282	-121.444	37.915
800	13.044	79.926	72.337	6.071	-118.732	-121.866	33.291
900	13.209	81.472	73.268	7.384	-119.284	-122.225	29.679
940	13.262	82.047	73.629	7.913	-119.540	-122.350	28.445
940	13.262	82.047	73.629	7.913	-120.225	-122.350	28.445
1000	13.332	82.870	74.159	8.711	-120.534	-122.476	26.766
1048	13.380	83.496	74.573	9.352	-120.781	-122.564	25.558
1048	13.380	83.496	74.573	9.352	-121.901	-122.564	25.558
1100	13.426	84.146	75.010	10.049	-122.118	-122.591	24.355
1200	13.499	85.317	75.821	11.395	-122.535	-122.616	22.330
1300	13.557	86.400	76.594	12.748	-12[illegible].954	-122.607	20.611
1400	13.604	87.406	77.330	14.106	-1[illegible]3.375	-122.564	19.132
1406	13.607	87.465	77.373	14.188	-123.400	-122.561	19.050
1406	13.607	87.465	77.373	14.188	-128.100	-122.561	19.050
1500	13.642	88.346	78.034	15.469	-128.497	-122.178	17.800
1600	13.674	89.228	78.706	16.835	-128.923	-121.742	16.628
1700	13.700	90.058	79.350	18.203	-129.353	-121.281	15.591
1800	13.722	90.841	79.967	19.575	-129.785	-120.794	14.666
1900	13.741	91.584	80.559	20.948	-130.221	-120.283	13.835
2000	13.757	92.289	81.128	22.323	-130.661	-119.746	13.085
2100	13.771	92.961	81.675	23.699	-131.106	-119.190	12.404
2200	13.784	93.602	82.203	25.077	-131.554	-118.610	11.782
2300	13.794	94.214	82.712	26.456	-132.006	-118.014	11.213
2400	13.804	94.802	83.204	27.836	-132.463	-117.396	10.690
2500	13.812	95.365	83.679	29.217	-132.925	-116.760	10.207
2600	13.819	95.907	84.139	30.598	-133.391	-116.103	9.759
2700	13.826	96.429	84.584	31.980	-133.862	-115.429	9.343
2800	13.832	96.932	85.016	33.363	-134.336	-114.735	8.955
2900	13.837	97.417	85.436	34.747	-134.815	-114.030	8.593
3000	13.842	97.887	85.843	36.131	-135.[illegible]98	-113.304	8.254
3100	13.846	98.340	86.239	37.515	-135.79[illegible]	-112.561	7.935
3200	13.850	98.780	86.624	38.900	-136.2[illegible]	-111.806	7.636
3300	13.854	99.206	86.999	40.285	-136.773	-111.034	7.353
3400	13.857	99.620	87.364	41.671	-137.272	-110.244	7.066
3500	13.860	100.027	87.720	43.057	-137.775	-109.440	6.833
3600	13.863	100.412	88.067	44.443	-138.282	-108.623	6.594
3700	13.865	100.792	88.406	45.829	-138.792	-107.796	6.367
3800	13.868	101.162	88.737	47.216	-139.305	-106.949	6.151
3900	13.870	101.522	89.060	48.603	-139.822	-106.088	5.945
4000	13.872	101.873	89.376	49.990	-140.342	-105.216	5.748
4100	13.874	102.216	89.685	51.377	-140.866	-104.335	5.561
4123.63	13.874	102.296	89.757	51.705	-140.990	-104.122	5.518
4123.63	13.874	102.296	89.757	51.705	-247.891	-104.126	5.518
4200	13.876	102.550	89.987	52.764	-248.[illegible]83	-101.452	5.279
4300	13.877	102.877	90.28[illegible]	54.152	-249.033	-97.947	4.978
4400	13.879	103.196	90.573	55.540	-249.694	-[illegible]4.424	4.690
4500	13.880	103.508	90.857	56.928	-250.361	-[illegible]0.891	4.414
4600	13.881	103.813	91.135	58.316	-251.039	-87.335	4.149
4700	13.883	104.111	91.408	59.704	-251.725	-83.766	3.895
4800	13.884	104.404	91.676	61.092	-252.422	-80.184	3.651
4900	13.885	104.690	91.939	62.481	-253.127	-76.595	3.416
5000	13.886	104.970	92.197	63.869	-253.845	-72.980	3.190
5100	13.887	105.245	92.450	65.258	-254.574	-69.356	2.972
5200	13.888	105.515	92.698	66.647	-255.315	-65.707	2.761
5300	13.889	105.780	92.943	68.036	-256.071	-62.060	2.559
5400	13.889	106.039	93.163	69.424	-256.846	-58.388	2.363
5500	13.890	106.294	93.419	70.813	-257.637	-54.702	2.174
5600	13.891	106.544	93.651	72.202	-258.452	-51.004	1.990
5700	13.892	106.790	93.879	73.592	-259.291	-47.283	1.813
5800	13.892	107.032	94.104	74.981	-260.164	-43.549	1.641
5900	13.893	107.269	94.325	76.370	-261.072	-39.804	1.474
6000	13.893	107.503	94.543	77.759	-262.024	-36.042	1.313

15 June 1963 MRP

URANIUM DIOXIDE (UO_2) (IDEAL MOLECULAR GAS) gfw = 270.07

ΔH_{f0}° = -116.0 kcal gfw^{-1}

$\Delta H_{f\,298.15}^{\circ}$ = -117 ± 10.0 kcal gfw^{-1}

$H_{298.15}^{\circ} - H_0^{\circ}$ = 2.629 kcal gfw^{-1}

$S_{298.15}^{\circ}$ = 68.2 cal deg K^{-1} gfw^{-1}

Vibration Levels

ω (cm^{-1})	ω (cm^{-1})
900	925
400	

Bond lengths and angles:

O - U distance = 1.96Å

O - U - O angle = 107 deg

Heat of Formation

Computed see volume 1, this study (section IVB32.4.2).

Heat Capacity and Entropy

Computed using the polyatomic gas program and the above estimated constants.

References

See volume 1, this study (section IVB32.4.2).

TABLE 206

VANADIUM DIOXIDE

IDEAL MOLECULAR GAS

O_2V

Reference State for Calculating ΔH_f^o, ΔF_f^o, and Log Kp: Solid V from 0° to 2190°K, Liquid V from 2190° to 3648°K, Gaseous V from 3648° to 6000°K; Gaseous O_2; Gaseous VO_2.

T, °K	C_p^o (cal/°K gfw)	S_T^o (cal/°K gfw)	$(H_T^o - H_{298}^o)/T$ (cal/°K gfw)	$H_T^o - H_{298}^o$ (Kcal/gfw)	ΔH_f^o (Kcal/gfw)	ΔF_f^o (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.785	-55.464	-55.464	INFINITE
298.15	12.266	59.912	59.912	0.000	-55.876	-57.076	41.836
300	12.290	59.988	59.913	0.023	-55.877	-57.084	41.584
400	13.260	63.671	60.408	1.305	-55.902	-57.480	31.404
500	13.793	66.693	61.372	2.660	-55.894	-57.875	25.296
600	14.104	69.237	62.476	4.056	-55.893	-58.272	21.224
700	14.299	71.427	63.602	5.477	-55.911	-58.668	18.316
800	14.429	73.346	64.703	6.914	-55.959	-59.059	16.133
900	14.521	75.051	65.760	8.362	-56.037	-59.443	14.434
1000	14.588	76.584	66.767	9.817	-56.147	-59.814	13.072
1100	14.639	77.977	67.723	11.279	-56.287	-60.174	11.955
1200	14.678	79.253	68.632	12.745	-56.457	-60.521	11.022
1300	14.709	80.429	69.495	14.214	-56.659	-60.852	10.230
1400	14.735	81.520	70.315	15.687	-56.890	-61.167	9.548
1500	14.755	82.537	71.096	17.161	-57.151	-61.462	8.955
1600	14.772	83.490	71.841	18.637	-57.442	-61.740	8.433
1700	14.786	84.386	72.553	20.115	-57.764	-61.999	7.970
1800	14.798	85.231	73.234	21.595	-58.115	-62.239	7.556
1900	14.809	86.032	73.887	23.075	-58.497	-62.458	7.184
2000	14.818	86.792	74.513	24.556	-58.909	-62.654	6.846
2100	14.825	87.515	75.115	26.038	-59.353	-62.831	6.539
2190	14.831	88.137	75.638	27.373	-59.777	-62.972	6.284
2190	14.831	88.137	75.638	27.373	-63.977	-62.972	6.284
2200	14.832	88.205	75.695	27.521	-64.015	-62.967	6.255
2300	14.838	88.864	76.253	29.005	-64.397	-62.912	5.978
2400	14.843	89.496	76.792	30.489	-64.785	-62.838	5.722
2500	14.848	90.102	77.312	31.973	-65.179	-62.748	5.485
2600	14.852	90.684	77.815	33.458	-65.576	-62.641	5.265
2700	14.856	91.245	78.302	34.944	-65.978	-62.523	5.061
2800	14.859	91.785	78.774	36.430	-66.384	-62.386	4.869
2900	14.862	92.306	79.232	37.916	-66.796	-62.239	4.690
3000	14.865	92.810	79.676	39.402	-67.212	-62.074	4.522
3100	14.867	93.298	80.108	40.889	-67.632	-61.893	4.363
3200	14.869	93.770	80.528	42.375	-68.058	-61.706	4.214
3300	14.871	94.227	80.936	43.862	-68.486	-61.499	4.073
3400	14.873	94.671	81.333	45.350	-6[illegible].918	-61.279	3.939
3500	14.875	95.103	81.721	46.837	-69.[illegible]55	-61.049	3.812
3600	14.876	95.522	82.098	48.325	-69.[illegible]95	-60.801	3.691
3647.68	14.877	95.717	82.275	49.034	-70.006	-60.684	3.636
3647.68	14.877	95.717	82.275	49.034	-179.880	-60.684	3.636
3700	14.878	95.929	82.466	49.812	-179.977	-58.969	3.483
3800	14.879	96.326	82.826	51.300	-180.175	-55.697	3.203
3900	14.880	96.713	83.177	52.788	-180.389	-52.417	2.937
4000	14.882	97.089	83.520	54.276	-180.618	-49.128	2.684
4100	14.883	97.457	83.856	55.764	-180.863	-45.843	2.444
4200	14.884	97.815	84.184	57.253	-181.124	-42.545	2.214
4300	14.885	98.166	84.505	58.741	-181.[illegible]01	-39.239	1.994
4400	14.886	98.508	84.819	60.230	-181.695	-35.931	1.785
4500	14.886	98.842	85.127	61.718	-182.005	-32.615	1.584
4600	14.887	99.170	85.429	63.207	-182.332	-29.288	1.391
4700	14.888	99.490	85.725	64.696	-182.676	-25.956	1.207
4800	14.888	99.803	86.015	66.185	-183.038	-22.617	1.030
4900	14.889	100.110	86.299	67.673	-183.419	-19.268	0.859
5000	14.890	100.411	86.579	69.162	-183.819	-15.916	0.696
5100	14.890	100.706	86.853	70.651	-184.239	-12.557	0.538
5200	14.891	100.995	87.122	72.140	-184.680	-9.180	0.386
5300	14.891	101.279	87.386	73.629	-185.145	-5.796	0.239
5400	14.892	101.557	87.646	75.119	-185.635	-2.411	0.098
5500	14.892	101.830	87.902	76.608	-186.153	0.994	-0.039
5600	14.893	102.099	88.153	78.097	-186.703	4.402	-0.172
5700	14.893	102.362	88.400	79.586	-187.288	7.821	-0.300
5800	14.893	102.621	88.643	81.076	-187.913	11.253	-0.424
5900	14.894	102.876	88.882	82.565	-188.585	14.706	-0.545
6000	14.894	103.126	89.117	84.054	-189.309	18.164	-0.662

15 September 1963 HLS

VANADIUM DIOXIDE (VO_2) (IDEAL MOLECULAR GAS) gfw = 82.95

ΔH_{f0}° = -55.464 kcal gfw^{-1}

$\Delta H_{f298.15}^\circ$ = -55.876 kcal gfw^{-1}

Point Group $D_{\infty h}$

$S_{298.15}^\circ$ = 59.912 cal deg K^{-1} gfw^{-1}

$H_{298.15}^\circ - H_0^\circ$ = 2.785 kcal gfw^{-1}

Vibrational Levels and Multiplicities

ω, cm^{-1}	ω, cm^{-1}
883.1 (1)	1126.8 (1)
293.8 (2)	

Bond lengths and angles:

V-O distance = 1.59 A

O-V-O angle = 180°

Moment of inertia:

I = 13.4312 x 10^{-39} gm cm^2 σ = 2

B_e = 0.20838 cm^{-1}

Heat of Formation

Based on Brewer and Rosenblatt[1] analysis of data by Berkowitz et al.[2]

Heat Capacity and Entropy

Estimated data were used to calculate thermodynamic functions.

References

1. Brewer, L. and G. Rosenblatt, Chem Rev. 61, 257 (1961).

2. Berkowitz, J. et al, J. Chem. Phys. 27, 87 (1957).

VANADIUM DIOXIDE (VO_2) (IDEAL MOLECULAR GAS) GFW = 82.95

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw			Kcal/gfw			Log K_p
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	
298.15	±1.000	±3.000	±3.000	±0.000	±10.000		
1000	±1.000	±4.210	±3.508	±0.702			
2000	±1.000	±4.903	±4.052	±1.702			
3000	±1.000	±5.309	±4.408	±2.702			
4000	±1.000	±5.596	±4.671	±3.702			
5000	±1.000	±5.820	±4.879	±4.702			
6000	±1.000	±6.002	±5.052	±5.702			

TABLE 207

TUNGSTEN DIOXIDE

CONDENSED PHASE

O_2W

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid W from 0° to 3650°K, Liquid W from 3650° to 5891°K, Gaseous W from 5891° to 6000°K, Gaseous O_2; Solid WO_2

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.077	-139.747	-139.747	INFINITE
298.15	13.320	12.080	12.080	0.000	-140.940	-127.596	93.526
300	13.350	12.162	12.080	0.025	-140.939	-127.513	92.889
400	15.172	16.266	12.618	1.459	-140.803	-123.041	67.223
500	16.160	19.767	13.707	3.030	-140.564	-118.636	51.853
600	16.860	22.827	14.994	4.700	-140.257	-114.277	41.623
700	17.425	25.493	16.293	6.440	-139.908	-109.977	34.335
800	17.916	27.884	17.596	8.230	-139.538	-105.713	28.878
900	18.366	30.026	18.859	10.050	-139.160	-101.524	24.652
1000	18.790	31.975	20.075	11.900	-138.770	-97.342	21.273
1100	19.197	33.767	21.240	13.780	-138.369	-93.242	18.524
1200	19.592	35.419	22.352	15.680	-137.963	-89.130	16.232
1300	19.978	36.965	23.419	17.610	-137.549	-85.107	14.307
1400	20.359	38.417	24.438	19.570	-137.126	-81.091	12.658
1500	20.736	39.804	25.417	21.580	-136.673	-77.103	11.233
1600	21.109	41.147	26.359	23.660	-136.173	-73.150	9.991
1700	21.479	47.468	27.268	25.840	-135.593	-69.231	8.900
1800	21.847	43.771	28.149	28.120	-134.935	-65.345	7.934
1900	22.214	45.058	29.005	30.500	-134.196	-61.499	7.074
2000	22.580	46.330	29.840	32.980	-133.379	-57.692	6.304

May 1962 CHW

TUNGSTEN DIOXIDE (WO_2) (CONDENSED PHASE) gfw = 215.86

$\Delta H^o_{f298.15} = -139.747$ Kcal gfw^{-1} $S^o_{298.15} = 12.080$ cal deg K^{-1} gfw^{-1}

$H^o_{298.15} - H^o_0$ 2.693 Kcal gfw^{-1}

$C^o_p = 15.49 + 3.58 \times 10^{-3} T - 2.80 \times 10^5 T^{-2}$ cal deg K^{-1} gfw^{-1}

$400\ ^oK \leq T \leq 1800\ ^oK$

Structure

WO_2 remains solid until disproportionation occurs.

Heat of Formation

Based on data by Mah.[1]

Heat Capacity and Entropy

Low temperature data by King *et al.*[2] High temperature data from same workers.

Melting and Vaporization

WO_2 does not melt, but rather disproportionates.

Further details in report by Barriault *et al.*[3]

References

1. Mah, A. D., J. Am. Chem. Soc. 81 1582 (1959).

2. King, E. G., *et al*, U.S. Bur. Mines. Rept. 5664 (1960).

3. Barriault, R., *et al*, ASD-TR-61-260 May (1962), Pt. 1.

TABLE 208

TUNGSTEN DIOXIDE **IDEAL MOLECULAR GAS** **O_2W**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid W from 0° to 3650°K, Liquid W from 3650° to 5891°K, Gaseous W from 5891° to 6000°K; Gaseous O_2; Gaseous WO_2.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.693	14.477	14.477	INFINITE
298.15	10.814	65.893	65.893	0.000	13.900	11.200	-8.209
300	10.835	65.960	65.893	0.020	13.896	11.183	-8.146
400	11.762	69.213	66.330	1.153	13.731	10.314	-5.635
500	12.370	71.908	67.184	2.362	13.608	9.466	-4.019
600	12.767	74.201	68.167	3.620	13.503	8.659	-3.154
700	13.035	76.190	69.174	4.911	13.403	7.846	-2.450
800	13.222	77.944	70.163	6.224	13.296	7.074	-1.932
900	13.356	79.509	71.116	7.554	13.184	6.285	-1.526
1000	13.455	80.922	72.027	8.894	13.064	5.546	-1.212
1100	13.530	82.208	72.895	10.244	12.935	4.777	-0.949
1200	13.588	83.388	73.721	11.600	12.797	4.067	-0.741
1300	13.634	84.477	74.507	12.961	12.642	3.318	-0.558
1400	13.671	85.489	75.256	14.326	12.470	2.605	-0.407
1500	13.701	86.433	75.970	15.695	12.282	1.908	-0.278
1600	13.726	87.318	76.652	17.066	12.073	1.222	-0.167
1700	13.747	88.151	77.304	18.440	11.847	0.551	-0.071
1800	13.764	88.937	77.929	19.816	11.601	-0.108	0.013
1900	13.779	89.682	78.528	21.193	11.[illegible]37	-0.751	0.086
2000	13.792	90.389	79.103	22.571	11.052	-1.378	0.151
2100	13.803	91.062	79.657	23.951	10.749	-1.991	0.207
2200	13.812	91.704	80.190	25.332	10.426	-2.592	0.257
2300	13.820	92.319	80.704	26.713	10.084	-3.176	0.302
2400	13.828	92.907	81.200	28.096	9.722	-3.744	0.341
2500	13.834	93.472	81.680	27.479	9.340	-4.298	0.376
2600	13.840	94.014	82.144	30.863	8.939	-4.836	0.406
2700	13.845	94.537	82.593	32.247	8.518	-5.357	0.434
2800	13.850	95.040	83.029	33.632	8.078	-5.863	0.458
2900	13.854	95.526	83.452	35.017	7.618	-6.354	0.479
3000	13.857	95.996	83.862	3[illegible].402	7.138	-6.828	0.497
3100	13.861	96.450	84.261	37.788	6.640	-7.282	0.513
3200	13.864	96.891	84.649	39.175	6.122	-7.725	0.528
3300	13.867	97.317	85.029	40.561	5.586	-8.158	0.540
3400	13.869	97.731	85.394	41.948	5.030	-8.558	0.550
3500	13.871	98.133	85.752	43.335	4.456	-8.946	0.559
3600	13.874	98.524	86.101	44.722	3.862	-9.317	0.566
3650	13.875	98.714	86.272	45.416	3.[illegible]	-9.497	0.569
3650	13.875	98.714	86.272	45.416	-4.8[illegible]	-9.497	0.569
3700	13.876	98.904	86.442	46.110	-5.13[illegible]	-9.561	0.565
3800	13.877	99.274	86.775	47.497	-5.730	-9.671	0.556
3900	13.879	99.635	87.100	48.885	-6.331	-9.770	0.547
4000	13.881	99.986	87.418	50.273	-6.935	-9.844	0.538
4100	13.882	100.329	87.729	51.661	-7.543	-9.918	0.529
4200	13.883	100.664	88.033	53.049	-8.155	-9.962	0.518
4300	13.885	100.990	88.330	54.438	-8.769	-9.989	0.508
4400	13.886	101.309	88.622	55.826	-9.389	-10.014	0.497
4500	13.887	101.622	88.907	57.215	-10.011	-10.026	0.487
4600	13.888	101.927	89.187	58.604	-10.638	-10.014	0.476
4700	13.889	102.225	89.461	59.993	-11.270	-9.992	0.465
4800	13.890	102.518	89.730	61.382	-11.908	-9.955	0.453
4900	13.891	102.804	89.994	62.771	-12.552	-9.908	0.442
5000	13.891	103.085	90.25[illegible]	64.160	-1[illegible].204	-9.845	0.430
5100	13.892	103.360	90.507	65.549	-13.865	-[illegible].772	0.419
5200	13.893	103.630	90.757	[illegible].938	-14.536	-9.682	0.407
5300	13.894	103.894	91.002	[illegible].327	-15.220	-9.577	0.395
5400	13.894	104.154	91.244	69.717	-15.918	-9.466	0.383
5500	13.895	104.409	91.481	71.106	-16.634	-9.339	0.371
5600	13.895	104.659	91.714	72.496	-17.371	-9.201	0.359
5700	13.896	104.905	91.943	73.885	-18.134	-9.040	0.347
5800	13.896	105.147	92.169	75.275	-18.928	-8.874	0.334
5891	13.897	105.364	92.371	76.540	-19.684	-8.701	0.323
5891	13.897	105.364	92.371	76.540	-211.949	-8.701	0.323
5900	13.897	105.385	92.391	76.665	-212.021	-8.396	0.311
6000	13.897	105.618	92.609	78.054	-212.869	-4.926	0.179

May 1962 CHW

TUNGSTEN DIOXIDE (WO_2) (IDEAL MOLECULAR GAS) gfw = 215.86

ΔH^o_{f0} = 14.477 Kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 13.900 Kcal gfw^{-1}

Point Group C_{2v}

$S^o_{298.15}$ = 65.893 cal $degK^{-1}$ gfw^{-1}

$H^o_{298.15} - H^o_0$ = 2.693 Kcal gfw^{-1}

Vibrational levels and multiplicities

ω, cm^{-1}	ω, cm^{-1}
794 (1)	812 (1)
351 (1)	

Bond lengths and angles:

W - O distance = 1.78 A

O - W - O Angle = 107 deg

Product of moments of inertia: $I_AI_BI_C$ = 8.80082×10^{-115} g^3 cm^6 $\sigma = 2$

Heat of Formation

Based on work of DeMaria *et al.*[1]

Heat Capacity and Entropy

Calculated using spectroscopic constants. See Barriault *et al*[2] for further details.

References

1. DeMaria, G., *et al*, J. Chem. Phys. 32 1373 (1960).

2. Barriault, R. *et al*, ASD-TR-61-260 May (1962), Pt. 1.

TABLE 209

ZIRCONIUM DIOXIDE — CONDENSED PHASE — O_2Zr

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p. Solid Zr from 0° to 2125°K, Liquid Zr from 2125° to 4644°K, Gaseous Zr from 4644° to 6000°K; Gaseous O_2; Monoclinic ZrO_2 from 0° to 1478°K, Tetragonal ZrO_2 from 1478° to 2973°K, Liquid ZrO_2 from 2973° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.091	-260.203	-260.203	INFINITE
298.15	13.397	12.120	12.120	0.000	-261.500	-247.732	181.584
300	13.447	12.203	12.120	0.025	-261.499	-247.647	180.402
400	15.260	16.353	12.674	1.472	-261.393	-243.042	132.786
500	16.196	19.868	13.771	3.049	-261.220	-238.474	104.232
600	16.787	22.877	15.044	4.700	-261.026	-233.942	85.209
700	17.214	25.498	16.354	6.401	-260.825	-229.444	71.632
800	17.555	27.820	17.645	8.140	-260.626	-224.975	61.457
900	17.845	29.905	18.893	9.910	-260.429	-220.530	53.549
1000	18.104	31.798	20.091	11.708	-260.235	-216.107	47.228
1100	18.342	33.535	21.235	13.530	-260.044	-211.704	42.060
1135	18.422	34.111	21.623	14.174	-259.976	-210.166	40.467
1135	18.422	34.111	21.623	14.174	-260.891	-210.166	40.467
1200	18.567	35.141	22.328	15.376	-260.755	-207.266	37.746
1300	18.781	36.636	23.372	17.243	-260.535	-202.818	34.095
1400	18.989	38.035	24.369	19.132	-260.300	-198.387	30.968
1478	19.147	39.069	25.118	20.619	-260.107	-194.941	28.824
1478	17.800	40.030	25.118	22.039	-258.687	-194.941	28.824
1500	17.800	40.293	25.339	22.431	-258.661	-193.994	28.264
1600	17.800	41.441	26.310	24.211	- 58.548	-189.687	25.909
1700	17.800	42.521	27.232	25.991	-258.441	-185.386	23.832
1800	17.800	43.538	28.110	27.771	-258.340	-181.092	21.987
1900	17.800	44.500	28.947	29.551	-258.244	-176.802	20.336
2000	17.800	45.413	29.748	31.331	-258.154	-172.518	18.851
2000	17.800	45.413	29.748	31.331	-258.154	-172.518	18.851
2100	18.437	46.297	30.515	33.143	-258.038	-168.239	17.508
2125	18.596	46.516	30.702	33.605	-258.000	-167.169	17.192
2125	18.596	46.516	30.702	33.605	-262.900	-167.169	17.192
2200	19.074	47.170	31.252	35.018	-262.771	-163.791	16.270
2300	19.712	48.032	31.963	36.957	-262.548	-159.300	15.136
2400	20.349	48.884	32.650	38.960	-262.267	-154.815	14.097
2500	20.986	49.728	33.317	41.027	-261.928	-150.348	13.143
2600	21.623	50.563	33.964	43.158	-261.529	-145.888	12.262
2700	22.260	51.391	34.594	45.352	-261.073	-141.453	11.449
2800	22.898	52.212	35.209	47.610	-260.557	-137.032	10.695
2900	23.535	53.027	35.809	49.931	-259.984	-132.627	9.995
2973	24.000	53.618	36.239	51.666	-259.528	-129.427	9.514
2973	24.000	62.027	36.239	76.666	-234.528	-129.427	9.514
3000	24.000	62.244	36.472	77.314	-234.353	-128.474	9.359
3100	24.000	63.031	37.316	79.714	-23[illegible]10	-124.951	8.809
3200	24.000	63.793	38.132	82.114	-23[illegible]72	-121.458	8.295
3300	24.000	64.531	38.921	84.514	-232.437	-117.980	7.813
3400	24.000	65.248	39.684	86.914	-231.807	-114.518	7.361
3500	24.000	65.943	40.425	89.314	-231.181	-111.077	6.936
3600	24.000	66.619	41.143	91.714	-230.559	-107.654	6.535
3700	24.000	67.277	41.841	94.114	-229.940	-104.250	6.157
3800	24.000	67.917	42.518	96.514	-229.325	-100.859	5.800
3900	24.000	68.540	43.178	98.914	-228.714	-97.486	5.463
4000	24.000	69.148	43.819	101.314	-228.106	-94.124	5.142
4100	24.000	69.741	44.444	103.714	-227.502	-90.784	4.839
4200	24.000	70.319	45.054	106.114	-226.902	-87.460	4.551
4300	24.000	70.884	45.648	108.514	-226.305	-84.142	4.276
4400	24.000	71.435	46.228	110.914	-225.713	-80.845	4.015
4500	24.000	71.975	46.794	113.314	-225.124	-77.558	3.767
4600	24.000	72.502	47.347	115.714	-224.540	-74.280	3.529
4644.05	24.000	72.731	47.58	116.772	-224.283	-72.840	3.428
4644.05	24.000	72.731	47.587	116.772	-359.737	-72.840	3.428
4700	24.000	73.018	47.888	118.114	-359.469	-69.388	3.226
4800	24.000	73.524	48.417	120.514	-358.997	-63.222	2.878
4900	24.000	74.019	48.934	122.914	-358.537	-57.057	2.545
5000	24.000	74.503	49.441	125.314	-358.089	-50.910	2.225
5100	24.000	74.979	49.937	127.714	-357.655	-44.776	1.919
5200	24.000	75.445	50.423	130.114	-357.236	-38.638	1.624
5300	24.000	75.902	50.899	132.514	-356.834	-32.514	1.341
5400	24.000	76.350	51.366	134.914	-356.450	-26.395	1.068
5500	24.000	76.791	51.825	137.314	-356.086	-20.287	0.806
5600	24.000	77.223	52.274	139.714	-355.748	-14.176	0.553
5700	24.000	77.648	52.716	142.114	-355.438	-8.078	0.310
5800	24.000	78.065	53.149	144.514	-355.161	-1.979	0.075
5900	24.000	78.476	53.575	146.914	-354.924	4.112	-0.152
6000	24.000	78.879	53.993	149.314	-354.733	10.210	-0.372

15 September 1963 — HLS

ZIRCONIUM DIOXIDE (ZrO_2) (CONDENSED PHASE) gfw = 123.22

$\Delta H^\circ_{f298.15}$ = -261.5 kcal gfw^{-1}

$S^\circ_{298.15}$ = 12.12 cal deg K^{-1} gfw^{-1}

T_t = 1478 °K

ΔH_t = 1.42 kcal gfw^{-1}

T_m = 2973 °K

ΔH_m = 25.0 kcal gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 2.091 kcal gfw^{-1}

$C^\circ_p = 16.64 + 1.80 \times 10^{-3}T - 3.36 \times 10^5 T^{-2}$ cal deg^{-1} gfw^{-1} 298.15 °K $\leq T \leq$ 1478 °K

C°_p = 17.80 cal deg K^{-1} gfw^{-1} 1478 °K $\leq T \leq$ 2000 °K

$C^\circ_p = 5.056 + .006372T$ cal deg K^{-1} gfw^{-1} 2000 °K $\leq T \leq$ 2973 °K

C°_p = 24.0 cal deg K^{-1} gfw^{-1} 2973 °K $\leq T \leq$ 6000 °K

ZrO_2 exists as monoclinic form below 1478°K and tetragonal above.

Heat of Formation

Combustion calorimetry was used by Humphrey.[1]

Heat Capacity and Entropy

Low temperature data from Kelley[2] and Kelley and King.[3] High temperature data to 2000°K from Kelley.[4] Data above 2000°K estimated.

Melting and Vaporization

Heat of melting was estimated.

References

1. Humphrey, G. L., J. Am. Chem. Soc. 76, 978 (1954).
2. Kelley, K. K., Ind. Eng. Chem. 36, 377 (1944).
3. Kelley, K. K., and E. G. King, Bur. of Mines. Bull. 592 (1961).
4. Kelley, K. K., Bur. of Mines Bull. 584 (1960).

ZIRCONIUM DIOXIDE (ZrO_2) (CONDENSED PHASE) GFW = 123.22

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw			Kcal/gfw			
	C°_p	S°_T	$-(F^\circ_T - H^\circ_{298})/T$	$H^\circ_T - H^\circ_{298}$	ΔH_f	ΔF_f	Log K_p
298.15	±0.300	±0.080	±0.080	±0.000	±2.000		
1000	±0.300	±0.443	±0.232	±0.211			
1478	±0.300	±0.560	±0.321	±0.354			
1478	±2.000	±0.560	±0.321	±0.354			
2000	±2.000	±1.165	±0.466	±1.398			
2973	±2.000	±1.958	±0.833	±3.344			
2973	±2.000	±4.649	±0.833	±11.344			
3000	±2.000	±4.667	±0.868	±11.398			
4000	±2.000	±5.242	±1.893	±13.398			
5000	±2.000	±5.689	±2.609	±15.398			
6000	±2.000	±6.053	±3.154	±17.398			

TABLE 210

ZIRCONIUM DIOXIDE IDEAL MOLECULAR GAS O_2Zr

Reference State for Calculating ΔH_f°, ΔF_f°, and Log Kp: Solid Zr from 0° to 2125°K, Liquid Zr from 2125° to 4644°K, Gaseous Zr from 4644° to 6000°K; Gaseous O_2; Gaseous ZrO_2.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.725	-81.794	-81.794	INFINITE
298.15	11.365	58.551	58.551	0.000	-82.457	-82.533	60.495
300	11.385	58.621	58.551	0.021	-82.460	-82.533	60.123
400	12.329	62.033	59.010	1.209	-82.613	-82.534	45.092
500	12.998	64.860	59.905	2.478	-82.748	-82.498	36.058
600	13.461	67.274	60.937	3.802	-82.881	-82.435	30.025
700	13.784	69.374	61.996	5.165	-83.018	-82.351	25.710
800	14.014	71.231	63.03[illegible]	6.556	-83.167	-82.245	22.467
900	14.182	72.892	64.041	7.966	-83.330	-82.120	19.941
1000	14.308	74.393	65.002	9.391	-83.509	-81.975	17.915
1100	14.405	75.761	65.919	10.827	-83.704	-81.813	16.254
1135	14.433	76.213	66.229	11.331	-83.776	-81.751	15.741
1135	14.433	76.213	66.229	11.331	-84.691	-81.751	15.741
1200	14.480	77.018	66.792	12.271	-84.817	-81.580	14.857
1300	14.540	78.179	67.624	13.722	-85.013	-81.303	13.668
1400	14.588	79.259	68.417	15.179	-85.210	-81.011	12.646
1500	14.627	80.267	69.174	16.639	-85.41[illegible]	-80.703	11.758
1600	14.660	81.212	69.897	18.104	-85.612	-80.383	10.979
1700	14.687	82.101	70.589	19.571	-85.818	-80.050	10.291
1800	14.710	82.941	71.252	21.041	-86.027	-79.705	9.677
1900	14.729	83.737	71.888	22.513	-86.239	-79.347	9.127
2000	14.746	84.493	72.500	23.987	-86.455	-78.979	8.630
2100	14.760	85.213	73.088	25.462	-86.676	-78.599	8.180
2125	14.764	85.388	73.232	25.831	-86.731	-78.502	8.073
2125	14.764	85.388	73.232	25.831	-91.631	-78.502	8.073
2200	14.773	85.900	73.655	26.939	-91.807	-78.035	7.752
2300	14.784	86.557	74.202	28.417	-92.045	-77.406	7.355
2400	14.794	87.186	74.730	29.895	-92.289	-76.764	6.990
2500	14.802	87.790	75.240	31.375	-92.537	-76.112	6.653
2600	14.810	88.371	75.734	32.856	-92.788	-75.447	6.342
2700	14.817	88.930	76.213	34.337	-93.045	-74.781	6.053
2800	14.823	89.469	76.677	35.819	-93.305	-74.099	5.783
2900	14.828	89.989	77.127	37.302	-93.570	-73.406	5.532
3000	14.833	90.492	77.564	38.785	-93.839	-72.707	5.296
3100	14.838	90.979	77.989	40.268	-94.113	-71.994	5.075
3200	14.842	91.450	78.402	41.752	-94.39[illegible]	-71.279	4.868
3300	14.845	91.906	78.804	43.237	-94.671	-70.551	4.672
3400	14.849	92.350	79.196	44.721	-94.957	-69.816	4.487
3500	14.852	92.780	79.578	46.[illegible]06	-95.246	-69.069	4.313
3600	14.855	93.199	79.951	47.692	-95.5[illegible]	-68.320	4.147
3700	14.857	93.606	80.314	49.177	-95.834	-67.557	3.990
3800	14.860	94.002	80.669	50.663	-96.133	-66.790	3.841
3900	14.862	94.388	81.016	52.149	-96.436	-66.011	3.699
4000	14.864	94.764	81.355	53.636	-96.741	-65.225	3.564
4100	14.866	95.131	81.687	55.122	-97.051	-64.437	3.435
4200	14.868	95.490	82.011	56.609	-97.364	-63.637	3.311
4300	14.870	95.839	82.329	58.096	-97.680	-62.827	3.193
4400	14.871	96.181	82.640	59.583	-98.001	-62.015	3.080
4500	14.873	9[illegible].515	82.944	61.070	-98.325	-61.190	2.972
4600	14.874	96.842	83.243	62.557	-98.654	-60.359	2.868
4644.05	14.875	96.984	83.373	63.212	-98.800	-59.[illegible]89	2.823
4644.05	14.875	96.984	83.373	63.212	-234.254	-59.[illegible]89	2.823
4700	14.875	97.162	83.536	6[illegible]45	-234.495	-57.890	2.692
4800	14.876	97.475	83.823	65.532	-234.936	-54.127	2.464
4900	14.878	97.782	84.105	67.020	-235.388	-50.352	2.246
5000	14.879	98.083	84.381	68.508	-235.852	-46.567	2.035
5100	14.880	98.377	84.653	69.996	-236.330	-42.784	1.833
5200	14.881	98.666	84.920	71.484	-236.823	-38.980	1.638
5300	14.881	98.950	85.182	72.972	-237.333	-35.170	1.450
5400	14.882	99.228	85.439	74.460	-237.861	-31.346	1.269
5500	14.883	99.501	85.692	75.948	-238.409	-27.512	1.093
5600	14.884	[illegible]9.769	85.941	77.437	-238.982	-23.668	0.924
5700	14.885	100.033	86.186	78.925	-239.584	-19.814	0.760
5800	14.885	100.292	86.427	80.413	-240.219	-15.948	0.601
5900	14.886	100.546	86.664	81.902	-240.893	-12.070	0.447
6000	14.886	100.796	86.898	83.391	-241.613	-8.177	0.298

15 September 1963 HLS

ZIRCONIUM DIOXIDE (ZrO_2) (IDEAL MOLECULAR GAS) gfw = 123.22

ΔH°_{f0} = -81.794 kcal gfw^{-1} $\Delta H^\circ_{f298.15}$ = -82.457 kcal gfw^{-1}

Point Group $D_{\infty h}$

$H^\circ_{298.15} - H^\circ_0$ = 2.725 kcal gfw^{-1} $S^\circ_{298.15}$ = 58.551 cal $degK^{-1}gfw^{-1}$

Vibrational Levels and Multiplicities

ω, cm^{-1}	ω, cm^{-1}
863.8 (1)	1003.9 (1)
261.8 (2)	

Bond lengths and angles:

Zr-O distance = 1.728 A

O-Zr-O Angle = 180°

Moments of inertia:

I = 15.8638 x 10^{-39} gcm^2 σ = 2

Heat of Formation

Data of Chupka, et al[1] was analyzed by third law method.

Heat Capacity and Entropy

Above basic input data was used.

Reference

1. Chupka, W. J., J. Berkowitz, M. Inghram, J. Chem. Phys. 26, 1207 (1957).

ZIRCONIUM DIOXIDE (ZrO_2) (IDEAL MOLECULAR GAS) GFW = 123.22

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C_p° (cal/°K gfw)	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f°	ΔF_f°	Log K_p
298.15	±1.000	±3.000	±3.000	±0.000	±7 000		
1000	±1.000	±4.210	±3.508	±0.702			
2000	±1.000	±4.903	±4.052	±1.702			
3000	±1.000	±5.309	±4.408	±2.702			
4000	±1.000	±5.596	±4.671	±3.702			
5000	±1.000	±5.820	±4.879	±4.702			
6000	±1.000	±6.002	±5.052	±5.702			

OSMIUM TRIOXIDE IDEAL MOLECULAR GAS **O_3Os**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p Solid Os from 0° to 3290°K Liquid Os from 3290° to 5270°K, Gaseous Os from 5270° to 6000°K; Gaseous O_2, Gaseous OsO_3.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-3.331	-66.809	-66.809	INFINITE
298.15	14.994	69.201	69.201	0.000	-67.800	-64.190	47.050
300	15.029	69.294	69.201	0.028	-67.803	-64.167	46.743
400	16.535	73.839	69.811	1.611	-67.885	-62.940	34.387
500	17.494	77.640	71.007	3.317	-67.883	-61.703	26.969
600	18.115	80.888	72.390	5.099	-67.853	-60.469	22.025
700	18.529	83.714	73.810	6.933	-67.811	-59.242	18.495
800	18.817	86.208	75.297	8.801	-67.775	-58.020	15.850
900	19.023	88.437	76.555	10.693	-67.748	-56.802	13.793
1000	19.175	90.449	77.846	12.604	-67.731	-55.587	12.148
1100	19.291	92.283	79.076	14.527	-67.728	-54.372	10.802
1200	19.380	93.965	80.248	16.461	-67.736	-53.158	9.681
1300	19.450	95.519	81.363	18.403	-67.759	-51.943	8.732
1400	19.507	96.963	82.427	20.351	-67.795	-50.726	7.918
1500	19.553	98.310	83.441	22.304	-67.843	-49.504	7.212
1600	19.591	99.573	84.410	24.261	-67.9[illegible]7	-48.281	6.595
1700	19.622	100.762	85.338	26.222	-67.98[illegible]	-47.052	6.049
1800	19.649	101.884	86.226	28.185	-68.078	-45.818	5.563
1900	19.671	102.947	87.078	30.151	-68.185	-44.577	5.127
2000	19.691	103.957	87.897	32.119	-68.307	-43.330	4.735
2100	19.707	104.918	88.685	34.089	-68.446	-42.078	4.379
2200	19.722	105.835	89.444	36.061	-68.599	-40.818	4.055
2300	19.735	106.712	90.176	38.033	-68.768	-39.555	3.758
2400	19.746	107.552	90.882	40.008	-68.952	-38.279	3.486
2500	19.756	108.355	91.566	41.983	-69.153	-37.001	3.234
2600	19.764	109.134	92.226	43.959	-69.368	-35.704	3.001
2700	19.772	109.880	92.867	45.935	-69.602	-34.410	2.785
2800	19.779	110.599	93.487	47.913	-69.848	-33.100	2.583
2900	19.785	111.293	94.089	49.891	-70.112	-31.783	2.395
3000	19.791	111.964	94.674	51.870	-70.389	-30.458	2.219
3100	19.796	112.613	95.242	53.849	-70.683	-29.117	2.053
3200	19.801	113.241	95.795	55.829	-70.992	-27.776	1.897
3290	19.805	113.790	96.279	57.612	-71.282	-26.555	1.764
3290	19.805	113.790	96.279	57.612	-78.849	-26.555	1.764
3300	19.806	113.851	96.333	57.810	-78.8[illegible]	-26.395	1.748
3400	19.809	114.442	96.857	[illegible].90	-79.260	-24.799	1.594
3500	19.813	115.016	97.367	61.771	-79.640	-23.187	1.448
3600	19.816	115.575	97.865	63.753	-80.025	-21.571	1.309
3700	19.819	116.118	98.351	65.735	-80.414	-19.941	1.178
3800	19.822	116.646	98.826	67.717	-80.810	-18.299	1.052
3900	19.824	117.161	99.290	69.699	-81.211	-16.653	0.933
4000	19.827	117.663	99.743	71.681	-81.617	-14.990	0.819
4100	19.829	118.153	100.186	73.664	-82.028	-13.319	0.710
4200	19.831	118.630	100.619	75.647	-82.445	-11.633	0.605
4300	19.833	119.097	101.044	77.630	-82.866	-9.943	0.505
4400	19.835	119.553	101.459	79.614	-83.295	-8.242	0.409
4500	19.836	119.999	101.866	81.597	-83.728	-6.533	0.317
4600	19.838	120.434	102.265	83.581	-84.168	-4.803	0.228
4700	19.839	120.861	102.656	85.565	-84.61[illegible]	-3.072	0.143
4800	19.841	121.279	103.040	87.549	-85.072	-1.332	0.061
4900	19.842	121.688	103.416	89.533	-85.538	0.[illegible]20	-0.019
5000	19.843	122.089	103.786	91.517	-86.015	[illegible].100	-0.095
5100	19.844	122.482	104.148	93.502	-86.505	3.952	-0.169
5200	19.845	122.867	104.505	95.486	-87.011	5.733	-0.241
5269.57	19.846	123.132	104.750	96.876	-87.374	6.979	-0.289
5269.57	19.846	123.132	104.750	96.876	-263.775	6.979	-0.289
5300	19.846	123.245	104.855	97.471	-263.930	8.544	-0.352
5400	19.847	123.616	105.199	99.455	-264.457	13.697	-0.554
5500	19.848	12[illegible].981	105.537	101.440	-265.012	18.696	-0.743
5600	19.849	124.338	105.870	103.425	-265.603	24.020	-0.937
5700	19.850	[illegible]4.690	106.197	105.410	-266.234	29.208	-1.120
5800	19.851	125.035	106.518	107.395	-266.916	34.411	-1.297
5900	19.851	125.374	106.835	109.380	-267.655	39.621	-1.468
6000	19.852	125.708	107.147	111.365	-268.463	44.844	-1.633

15 September 1962 CHW

OSMIUM TRIOXIDE (OsO_3) (IDEAL MOLECULAR GAS) gfw = 238.2

ΔH^o_{f0} = -66.809 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = -67.800 kcal gfw^{-1}

Point Group = D_{3h}

$S^o_{298.15}$ = 69.201 cal deg K^{-1}gfw^{-1}

$H^o_{298.15}-H^o_0$ = 3.331 kcal gfw^{-1}

Vibrational Levels and Multiplicities

ω, cm^{-1}	ω, cm^{-1}
764 (1)	811 (2)
291 (1)	292 (2)

Bond lengths and angles:

Os-O distance = 185 Å

O-Os-O angle = 120°

Product of moments of inertia:

$I_A I_B I_C = 5.072420 \times 10^{-114} g^3 cm^6 \quad \sigma = 6$

Heat of Formation

Based on Grimley *et al*[1] mass-spectrometric data.

Heat Capacity and Entropy

Spectroscopic data estimated. See volume 1, this study (section IVB18.4.3) for details.

Reference

1. Grimley, R. T., R. P. Burns, and M. G. Inghram, J. Chem. Phys. 33, 308 (1960).

TABLE 212

TITANIUM SESQUIOXIDE **CONDENSED PHASE** **O_3Ti_2**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ti from 0° to 1950°K, Liquid Ti from 1950° to 3550°K, Gaseous Ti from 3550° to 6000°K; Gaseous O_2; Solid Ti_2O_3 from 0° to 2093°K, Liquid Ti_2O_3 from 2093° to 6000°K.

T, °K	cal/°K gfw			Kcal/gfw			Log K_p
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	
0	0.000	0.000	INFINITE	-3.435	-361.423	-361.423	INFINITE
298.15	23.267	18.830	18.830	0.000	-363.400	-342.726	251.213
300	23.366	18.974	18.830	0.043	-363.398	-342.598	249.570
400	28.718	26.429	19.811	2.647	-363.099	-335.698	183.408
473	32.625	31.562	21.231	4.886	-362.600	-330.757	152.819
473	30.736	32.016	21.231	5.101	-362.385	-330.757	152.819
500	31.250	33.737	21.860	5.938	-362.203	-328.934	143.770
600	32.627	39.566	24.337	9.138	-361.483	-322.348	117.409
700	33.508	44.666	26.884	12.447	-360.727	-315.885	98.619
800	34.126	49.183	29.395	15.831	-359.960	-309.532	84.556
900	34.591	53.231	31.822	19.268	-359.194	-303.272	73.641
1000	34.960	56.895	34.149	22.746	-358.438	-297.098	64.928
1100	35.267	60.242	36.371	26.258	-357.693	291.002	57.814
1155	35.417	61.966	37.549	28.201	-357.287	-287.676	54.432
1155	35.417	61.966	37.549	28.201	-359.187	-287.676	54.432
1200	35.532	63.322	38.491	29.798	-358.857	-284.897	51.884
1300	35.766	66.176	40.512	33.363	-358.133	-278.765	46.862
1400	35.980	68.834	42.441	36.950	-357.422	-272.686	42.566
1500	36.177	71.323	44.284	40.558	-356.719	-266.658	38.850
1600	[illegible]	73.[illegible]64	46.048	44.185	-356.030	-260.678	35.605
1700	36.537	75.874	47.738	47.830	-355.351	-254.738	32.747
1800	36.705	77.967	49.360	51.493	-354.684	-248.840	30.212
1900	36.867	79.956	50.918	55.171	-354.029	-242.975	27.947
1950	36.947	80.915	51.675	57.017	-353.704	-240.056	26.903
1950	36.947	80.915	51.675	57.017	-361.104	-240.056	26.903
2000	37.025	81.851	52.418	58.866	-360.734	-236.958	25.892
2093	37.168	83.537	53.764	62.316	-360.035	-231.220	24.143
2093	37.500	98.348	53.764	93.316	-329.035	-231.220	24.143
2100	37.500	98.474	53.912	93.578	-328.981	-230.891	24.028
2200	37.500	100.218	55.978	97.328	-328.197	-226.240	22.474
2300	37.500	101.885	57.938	101.078	-327.421	-221.625	21.058
2400	37.500	103.481	59.803	104.828	-326.654	-217.040	19.763
2500	37.500	105.012	61.580	108.578	-325.896	-212.489	18.575
2600	37.500	106.483	63.279	112.328	-325.144	-207.963	17.480
2700	37.500	107.898	64.906	116.078	-324.401	-203.475	16.469
2800	37.500	109.262	66.466	11[illegible]	-323.664	99.006	15.532
2900	37.500	110.578	67.964	123.578	-322.936	[illegible]4.566	14.662
3000	37.500	111.849	69.406	127.328	-322.214	-[illegible]70.154	13.852
3100	37.500	113.078	70.795	131.078	-321.500	-185.762	13.096
3200	37.500	114.269	72.135	134.828	-320.79[illegible]	-181.398	12.388
3300	37.500	115.42[illegible]	73.430	138.578	-320.090	-177.049	11.725
3400	37.500	116.542	74.681	142.328	-319.395	-172.723	11.102
3500	37.500	117.630	75.893	146.078	-318.706	-168.420	10.516
3550	37.500	118.161	76.484	147.953	-318.363	-166.276	10.236
3550	37.500	118.161	76.484	147.953	-523.277	-166.276	10.236
3600	37.500	118.686	77.067	149.828	-522.947	-161.251	9.789
3700	37.500	119.713	78.206	153.578	-522.309	-151.212	8.931
3800	37.500	120.713	79.311	157.328	-521.704	-141.186	8.120
3900	37.500	121.688	80.385	161.078	-521.134	-131.184	7.351
4000	37.500	12[illegible].637	81.430	164.828	-520.592	-121.190	6.621
4100	37.500	123.563	82.446	168.578	-520.082	-111.2[illegible]9	5.928
4200	37.500	124.467	83.436	172.328	-519.602	-101.[illegible]	5.268
4300	37.500	125.349	84.401	17[illegible]78	-519.150	-91.283	4.639
4400	37.500	126.211	85.341	179.328	-518.728	-81.334	4.040
4500	37.500	127.054	86.259	183.578	-518.333	-71.409	3.468
4600	37.500	127.878	87.154	187.328	-517.965	-61.465	2.920
4700	37.500	128.684	88.030	191.078	-517.626	-51.555	2.397
4800	37.500	129.474	88.885	194.828	-517.315	-41.634	1.896
4900	37.500	130.247	89.721	198.578	-517.030	-31.721	1.415
5000	37.500	131.005	90.539	202.328	-516.774	-21.820	0.954
5100	37.500	131.747	91.340	206.078	-516.549	-11.923	0.511
5200	37.500	1[illegible].476	92.124	209.828	-516.353	-2.031	0.085
5300	37.500	133.190	92.892	213.578	-516.190	7.868	-0.324
5400	37.500	133.891	93.645	217.328	-516.064	17.748	-0.718
5500	37.500	134.57[illegible]	94.383	221.078	-515.976	27.647	-1.099
5600	37.500	135.255	95.107	224.828	-515.932	37.524	-1.464
5700	37.500	135.919	95.817	228.578	-515.936	47.422	-1.818
5800	37.500	136.571	96.514	232.328	-515.998	57.312	-2.159
5900	37.500	137.212	97.198	236.078	-516.124	67.211	-2.490
6000	37.500	137.842	97.870	239.828	-516.323	77.138	-2.809

31 December 1963 HLS

TITANIUM SESQUIOXIDE (Ti_2O_3) (CONDENSED PHASE) gfw = 143.80

$\Delta H^o_{f298.15} = -363.4$ kcal gfw^{-1} | $S^o_{298.15} = 18.83$ cal degK^{-1}gfw^{-1}

$T_t = 473^oK$ | $\Delta H_t = 0.215$ kcal gfw^{-1}

$T_m = 2093^oK$ | $\Delta H_m = 31.0$ kcal gfw^{-1}

$H^o_{298.15} - H^o_0 = 3.435$ kcal gfw^{-1}

$C^o_p = 7.31 + 53.52\times10^{-3}T$ cal degK^{-1}gfw^{-1} $\quad 298.15^oK \leq T \leq 473^oK$

$C^o_p = 34.68 + 1.30\times10^{-3}T - 10.20\times10^5T^{-2}$ cal degK^{-1}gfw^{-1} $\quad 473^oK \leq T \leq 2093^oK$

$C^o_p = 37.5$ cal degK^{-1}gfw^{-1} $\quad 2093^oK \leq T \leq 6000^oK$

Structure

Ti_2O_3 has hexagonal structure with narrow homogeneity range according to Andersson et al.[1]

Heat of Formation

Combustion calorimetric data of Mah et al[2] used.

Heat Capacity and Entropy

Low-temperature data by Shomate.[3] High-temperature data by Naylor[4] to 1750°K extrapolated to melting point. Data at higher temperatures estimated.

Melting and Vaporization

Melting point from Brauer and Littke.[5] Heat of fusion estimated.

References

1. Andersson, S. et al, Acta Chem. Scand. 11, 1653 (1957).
2. Mah, A. et al, U.S. Bur. Mines, Rept. 5316 (1957).
3. Shomate, C., J. Am. Chem. Soc. 68, 310 (1946).
4. Naylor, B., J. Am. Chem. Soc. 68, 1077 (1946).
5. Brauer, G. and W. Littke, J. Inorg. Nuclear Chem. 16, 67 (1960).

TITANIUM SESQUIOXIDE (Ti_2O_3) (CONDENSED PHASE) GFW = 143.80

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal °K gfw^{-1} C_p	S_T	$-(F_T - H_{298})/T$	$H_T - H_{298}$	kcal gfw^{-1} ΔH_f	ΔF_f	Log K_p
298.15	± 0.400	± 0.090	± 0.090	± 0.000	±1.500		
473	± 0.400	± 0.275	± 0.127	± 0.070			
473	± 1.000	± 0.380	± 0.127	± 0.120			
1000	± 1.000	± 1.129	± 0.482	± 0.647			
2000	± 1.000	± 1.822	± 0.999	± 1.647			
2093	± 1.000	± 1.868	± 1.036	± 1.740			
2093	± 5.000	± 5.690	± 1.036	± 9.740			
3000	± 5.000	± 7.490	± 2.732	± 14.275			
4000	± 5.000	± 8.928	± 4.110	± 19.275			
5000	± 5.000	± 10.044	± 5.189	± 24.275			
6000	± 5.000	± 10.956	± 6.076	± 29.275			

TABLE 213

TUNGSTEN TRIOXIDE **CONDENSED PHASE** **O_3W**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log Kp: Solid W; Gaseous O_2; Solid WO_3 from 0° to 1745°K, Liquid WO_3 from 1745° to 2000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-2.962	-200.115	-200.115	INFINITE
298.15	17.600	18.150	18.150	0.000	-201.460	-182.620	133.858
300	17.650	18.259	18.150	0.033	-201.458	-182.503	132.947
400	19.849	23.663	18.870	1.917	-201.226	-176.205	96.269
500	21.182	28.249	20.299	3.975	-200.866	-169.999	74.303
600	22.060	32.193	21.961	6.139	-200.443	-163.852	59.680
700	22.724	35.645	23.674	8.380	-199.982	-157.803	49.266
800	23.273	38.716	25.366	10.680	-199.501	-151.797	41.467
900	23.756	41.486	27.005	13.033	-198.996	-145.130	35.241
1000	24.198	44.012	28.582	15.430	-198.473	-139.986	30.592
1050	24.408	45.197	29.344	16.646	-198.207	-137.085	28.532
1050	23.678	45.587	29.344	17.056	-197.797	-137.085	28.532
1100	23.815	46.691	30.106	18.243	-197.559	-134.200	26.662
1200	24.090	48.775	31.577	20.638	-197.082	-128.438	23.391
1300	24.365	50.714	32.975	23.061	-196.603	-122.764	20.638
1400	24.640	52.530	34.308	25.511	-196.122	-117.107	18.280
1500	24.915	54.239	35.580	27.989	-195.677	-111.479	16.242
1600	25.190	55.856	36.797	30.494	-195.150	-105.883	14.462
1700	25.465	57.391	37.963	33.027	-194.659	-100.320	12.896
1745	25.589	58.058	38.473	34.176	-194.440	-97.833	12.252
1745	31.500	68.115	38.473	51.726	-176.890	-97.833	12.252
1800	31.500	69.093	39.394	53.458	-176.294	-95.344	11.576
1900	31.500	70.795	41.001	56.608	-175.232	-90.871	10.452
2000	31.500	72.411	42.532	59.758	-174.195	-86.458	9.447

May 1962 CHW

$\Delta H^o_{f298.15}$ = -201.460 Kcal gfw^{-1}

$S^o_{298.15}$ = 18.15 cal deg K^{-1} gfw^{-1}

T_t = 1050 °K

ΔH_t = 0.410 Kcal gfw^{-1}

T_m = 1745 °K

ΔH_m = 17.550 Kcal gfw^{-1}

$H^o_{298.15} - H^o_0$ 2.962 Kcal gfw^{-1}

$C^o_p = 21.26 + 3.38 \times 10^{-3} T - 4.42 \times 10^5 T^{-2}$ cal deg K^{-1} gfw^{-1}

$400\ ^oK \leq T \leq 1050\ ^oK$

$C^o_p = 20.79 + 2.75 \times 10^{-3} T$ cal deg K^{-1} gfw^{-1} $1050°K \leq T \leq 1745°K$

$C^o_p = 31.5$ cal deg K^{-1} gfw^{-1} $1745^oK \leq T \leq 2000°K$

Structure

The low temperature form is monoclinic, high temperature form is tetragonal.

Heat of Formation

Combustion calorimetry value by Mah[1] was used.

Heat Capacity and Entropy

Low temperature data by King et al[2]. High temperature data also based on King et al.[2] Details of analysis given by Barriault et al.[3]

Melting and Vaporization

Heat of melting from King et al.[2]

References

1. Mah, A. D., J. Am. Chem. Soc. 81, 1582 (1959).
2. King, E. G., et al, Bur. Mines. Rept. 5664 (1960).
3. Barriault, R., et al, ASD-TR-61-260 (May 1962), Pt. I.

TABLE 214

TUNGSTEN TRIOXIDE — IDEAL MOLECULAR GAS — O_3W

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p. Solid W from 0° to 3650°K, Liquid W from 3650° to 5891°K, Gaseous W from 5891° to 6000°K; Gaseous O_2; Gaseous WO_3.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-3.296	-64.089	-64.089	INFINITE
298.15	14.936	68.626	68.626	0.000	-65.100	-61.309	44.939
300	14.972	68.718	68.626	0.028	-65.103	-61.286	44.645
400	16.514	73.253	69.234	1.608	-65.175	-59.990	32.776
500	17.487	77.051	70.428	3.311	-65.170	-58.703	25.658
600	18.113	80.299	71.809	5.094	-65.128	-57.401	20.907
700	18.530	83.124	73.228	6.927	-65.075	-56.131	17.524
800	18.818	85.618	74.624	8.795	-65.026	-54.843	14.982
900	19.025	87.847	75.[illegible]72	10.688	-64.981	-53.591	13.013
1000	19.177	89.860	77.262	12.598	-64.945	-52.306	11.431
1100	19.292	91.693	78.492	14.522	-64.920	-51.065	10.145
1200	19.381	93.376	79.663	16.456	-64.904	-49.782	9.066
1300	19.452	94.930	80.778	18.398	-64.906	-48.549	8.161
1400	19.508	96.374	81.841	20.346	-64.927	-47.292	7.382
1500	19.554	97.721	82.855	22.299	-64.967	-46.031	6.706
1600	19.592	98.985	83.824	24.256	-65.028	-44.766	6.115
1700	19.623	100.173	84.752	26.217	-65.[illegible]9	-43.500	5.592
1800	19.649	101.296	85.640	28.181	-65.211	-42.226	5.127
1900	19.672	102.359	86.492	30.147	-65.333	-40.943	4.709
2000	19.691	103.368	87.311	32.115	-65.478	-39.656	4.333
2100	19.708	104.329	88.099	34.085	-65.644	-38.359	3.992
2200	19.722	105.247	88.857	36.057	-65.832	-37.055	3.681
2300	19.735	106.124	89.589	38.029	-66.041	-35.742	3.396
2400	19.746	106.964	90.296	40.004	-66.271	-34.426	3.135
2500	19.756	107.770	90.979	41.979	-66.525	-33.093	2.893
2600	19.765	108.545	91.639	43.955	-66.800	-31.749	2.669
2700	19.772	109.291	92.279	45.932	-67.098	-30.391	2.460
2800	19.779	110.010	92.900	47.909	-67.416	-29.028	2.266
2900	19.786	110.705	93.502	49.887	-67.757	-27.652	2.084
3000	19.791	111.375	94.087	51.866	-68.119	-26.265	1.913
3100	19.797	112.024	94.655	53.846	-68.502	-24.856	1.752
3200	19.801	112.653	95.208	55.826	-68.908	-23.450	1.601
3300	19.805	113.262	95.745	57.806	-69.332	-22.014	1.458
3400	19.809	113.854	96.269	59.787	-69.780	-20.577	1.323
3500	19.813	114.428	96.780	61.768	-70.24[illegible]	-19.117	1.194
3600	19.816	114.986	97.278	63.749	-70.73[illegible]	-17.647	1.071
3650	19.818	115.258	97.521	64.740	-70.987	-16.907	1.012
3650	19.818	115.258	97.521	64.740	-79.382	-16.907	1.012
3700	19.819	115.529	97.764	65.731	-79.626	-16.058	0.948
3800	19.822	116.058	98.239	67.713	-80.[illegible]21	-14.334	0.824
3900	19.824	116.573	98.702	69.695	-80.623	-12.589	0.705
4000	19.827	117.075	99.155	71.678	-81.128	-10.836	0.592
4100	19.829	117.564	99.598	73.661	-81.639	-9.077	0.484
4200	19.831	118.042	100.032	75.644	-82.156	-7.300	0.380
4300	19.833	118.509	100.456	77.627	-82.677	-5.504	0.280
4400	19.835	118.965	100.871	79.610	-83.207	-3.696	0.184
4500	19.836	119.410	101.279	81.594	-83.737	-1.899	0.092
4600	19.838	119.846	101.677	83.578	-84.279	-0.060	0.003
4700	19.839	120.273	102.069	85.561	-84.828	1.772	-0.082
4800	19.841	120.691	102.452	87.545	-85.384	3.634	-0.165
4900	19.842	121.100	102.829	89.530	-85.949	5.483	-0.245
5000	19.843	121.501	103.198	91.514	-86.526	[illegible].365	-0.322
5100	19.844	121.894	103.561	93.498	-87.117	9.241	-0.396
5200	19.845	122.279	103.917	95.483	-87.722	11.149	-0.469
5300	19.846	122.657	104.267	97.467	-88.348	13.054	-0.538
5400	19.847	123.028	104.611	99.452	-88.995	14.980	-0.606
5500	19.848	123.392	104.949	101.437	-89.667	16.918	-0.672
5600	19.849	123.750	105.282	103.422	-90.373	18.855	-0.736
5700	19.850	124.101	105.609	105.407	-91.116	20.822	-0.798
5800	19.851	124.447	105.931	107.392	-91.907	22.800	-0.859
5891	19.852	124.755	106.219	109.198	-92.677	24.613	-0.913
5891	19.852	124.755	106.219	109.198	-284.942	24.613	-0.913
5900	19.852	124.786	106.247	109.377	-285.015	25.087	-0.929
6000	19.852	125.120	106.559	111.362	-285.900	30.360	-1.106

May 1962 — CHW

TUNGSTEN TRIOXIDE (WO_3) (IDEAL MOLECULAR GAS) gfw = 231.86

ΔH^o_{f0} = 64.089 Kcal gfw^{-1}

$\Delta H^o_{f298.15}$ -65.100 Kcal gfw^{-1}

Point Group D_{3h}

$S^o_{298.15}$ 68.626 cal degK^{-1} gfw^{-1}

$H^o_{298.15} - H^o_0$ = 3.296 Kcal gfw^{-1}

Vibrational levels and multiplicities

ω, cm^{-1}	ω, cm^{-1}
780 (1)	791 (2)
298 (1)	314 (2)

Bond lengths and angles

W - O distance = 1.78 A

O - W - O Angle 120 deg

Product of moments of inertia $I_A I_B I_C$ 4 024423 x 10^{-114} g^3 cm^6

Heat of Formation

Based on work of DeMaria et al.[1]

Heat Capacity and Entropy

Calculated using above estimated spectroscopic constants Details are given by Barriault et al.[2]

References

1. DeMaria, G. et al, J. Chem Phys. 32, 1373 (1960)
2. Barriault, R et al, ASD-TR-61-260 (May 1962), Pt. I.

TABLE 215

OSMIUM TETROXIDE IDEAL MOLECULAR GAS **O_4Os**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log Kp: Solid Os from 0° to 3290°K, Liquid Os from 3290° to 5270°K, Gaseous Os from 5270° to 6000°K, Gaseous O_2; Gaseous OsO_4

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-3.689	-78.829	-78.829	INFINITE
298.15	17.727	70.800	70.800	0.000	-80.500	-70.061	51.353
300	17.776	70.909	70.800	0.033	-80.504	-69.996	50.989
400	19.994	76.345	76.345	1.928	-80.629	-66.469	36.315
500	21.530	80.983	72.965	4.000	-80.618	-62.928	27.504
600	22.581	85.007	74.644	6.218	-80.539	-59.396	21.634
700	23.312	88.546	76.383	8.514	-80.423	-55.882	17.446
800	23.832	91.695	78.103	10.873	-80.295	-52.385	14.310
900	24.211	94.525	79.774	13.276	-80.164	-48.905	11.875
1000	24.495	97.091	81.379	15.712	-80.036	-45.436	9.930
1100	24.712	99.436	82.915	18.173	-79.915	-41.981	8.341
1200	24.881	101.594	84.383	20.653	-79.801	-38.538	7.018
1300	25.015	103.591	85.785	23.148	-79.699	-35.107	5.902
1400	25.123	105.449	87.124	25.655	-79.608	-31.679	4.945
1500	25.211	107.185	88.404	28.172	-79.527	-28.258	4.117
1600	25.284	108.815	89.629	30.697	-79.462	-24.844	3.393
1700	25.345	[illegible]	90.804	33.228	-79.411	-21.432	2.755
1800	25.397	[illegible]	91.930	35.765	[illegible]	-18.022	2.188
1900	25.441	[illegible]	93.012	38.307	[illegible]	-14.614	1.681
2000	25.478	114.480	94.053	40.853	-79.347	-11.204	1.224
2100	25.511	115.724	95.056	43.403	-79.359	-7.798	0.812
2200	25.539	116.911	96.023	45.955	-79.387	-4.389	0.436
2300	[illegible]	[illegible]	96.956	48.511	-79.430	-0.982	0.093
2400	25.585	119.136	97.857	51.068	-79.493	2.432	-0.221
2500	25.605	[illegible]	98.729	53.628	-79.573	5.845	-0.511
2600	25.622	121.185	99.574	56.189	-79.670	9.268	-0.779
2700	25.637	122.152	100.392	58.752	-79.785	12.688	-1.027
2800	25.651	123.085	101.186	61.316	-79.916	16.117	-1.258
2900	25.663	123.985	101.957	63.882	-80.066	19.547	-1.473
3000	25.674	124.855	102.706	66.449	-80.231	22.985	-1.674
3100	25.684	125.697	103.434	69.017	-80.415	26.434	-1.864
3200	25.693	126.513	104.143	71.586	-80.616	29.878	-2.040
3290	25.701	127.225	104.763	73.898	-80.811	32.992	-2.191
3290	25.701	127.225	104.763	73.898	-88.378	32.992	-2.191
3300	25.702	127.304	104.832	74.155	-88.403	33.363	-2.209
3400	25.709	128.071	105.505	76.726	-88.672	37.055	-2.382
3500	25.716	128.817	106.160	79.297	-88.94[illegible]	40.761	-2.545
3600	25.723	129.541	106.800	81.869	-89.234	44.467	-2.699
3700	25.729	130.246	107.424	84.442	-89.522	48.186	-2.846
3800	25.734	130.942	108.033	87.015	-89.819	51.919	-2.986
3900	25.739	131.601	108.629	89.589	-90.123	55.649	-3.118
4000	25.744	132.252	109.212	92.163	-90.433	59.392	-3.245
4100	25.748	132.888	109.781	94.737	-90.751	63.143	-3.366
4200	25.752	133.509	110.339	97.313	-91.075	66.903	-3.481
4300	25.756	134.115	110.885	99.888	-91.406	70.671	-3.592
4400	25.760	134.707	111.420	102.464	-91.746	74.442	-3.697
4500	25.763	135.286	111.944	105.040	-92.092	78.220	-3.799
4600	25.766	135.852	112.457	107.616	-92.448	82.023	-3.897
4700	25.769	136.406	112.961	110.193	-92.813	85.819	-3.990
4800	25.771	136.949	113.455	112.770	-93.190	89.626	-4.081
4900	25.774	137.480	113.940	115.347	[illegible]	93.440	-4.167
5000	25.776	138.001	114.416	117.925	-93.983	97.265	-4.251
5100	25.779	138.511	114.883	[illegible]	-94.405	[illegible]	-4.332
5200	25.781	139.012	115.343	[illegible]	-94.847	104.937	-4.410
5269.57	25.782	139.356	115.659	124.896	-95.170	107.623	-4.463
5269.57	25.782	139.356	115.659	124.886	-271.571	107.623	-4.463
5300	25.783	139.503	115.794	125.659	-271.709	109.807	-4.528
5400	25.785	139.985	116.237	128.237	-272.196	117.021	-4.736
5500	25.786	140.458	116.673	130.816	-272.700	124.078	-4.930
5600	25.788	140.923	117.102	133.394	-273.261	131.460	-5.130
5700	25.790	141.379	117.524	135.973	-273.874	138.705	-5.318
5800	25.791	141.828	117.939	138.552	-274.554	145.961	-5.500
5900	25.793	142.269	118.348	141.131	-275.310	153.228	-5.676
6000	25.794	142.707	118.750	143.711	-276.155	160.514	-5.846

15 September 1962 CHW

OSMIUM TETROXIDE (OsO_4) (IDEAL MOLECULAR GAS) gfw = 254.2

ΔH^{o}_{f0} = -78.829 kcal gfw^{-1}

$\Delta H^{o}_{f298.15}$ = -80.500 kcal gfw^{-1}

Point Group = T_d

$S^{o}_{298.15}$ = 70.800 cal deg K^{-1}gfw^{-1}

$H^{o}_{298.15}-H^{o}_{0}$ = 3.689 kcal gfw^{-1}

Vibrational Levels and Multiplicities

ω, cm^{-1}	ω, cm^{-1}
971 (1)	959.7 (3)
328 (2)	328 (3)

Bond lengths and angles:

Os-O distance = 185 Å

Product of moments of inertia:

$I_AI_BI_C$ = 1.4250638 x $10^{-113}g^3cm^6$ σ = 12

Heat of Formation

Coughlin's value adopted.[1]

Heat Capacity and Entropy

Determined from spectroscopic data. See volume 1, this study (section IVB18.4.4) for details.

Reference

1. Coughlin, J. P., U S. Bur. Mines, Bull. 542 (1954).

TABLE 216

TANTALUM PENTOXIDE **CONDENSED PHASE** **O_5Ta_2**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ta from 0° to 3270°K, Liquid Ta from 3270° to 5706°K, Gaseous Ta from 5706° to 6000°K, Gaseous O_2; Solid Ta_2O_5 from 0° to 2150°K, Liquid Ta_2O_5 from 2150° to 6000°K.

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-5.495	-486.291	-486.291	INFINITE
298.15	32.296	34.200	34.200	0.000	-488.700	-456.453	334.573
300	32.390	34.400	34.201	0.060	-488.694	-456.253	332.364
400	35.924	44.261	35.521	3.496	-488.271	-445.496	243.396
500	37.912	52.508	38.117	7.195	-487.666	-434.869	190.072
600	39.292	59.548	41.117	11.059	-486.976	-424.373	154.570
700	40.384	65.689	44.198	15.044	-486.231	-413.998	129.250
800	41.323	71.144	47.231	19.131	-485.451	-403.732	110.289
900	42.173	76.061	50.166	23.306	-484.631	-393.565	95.566
1000	42.968	80.546	52.983	27.563	-483.776	-383.491	83.808
1100	43.727	84.677	55.679	31.898	-482.877	-373.506	74.205
1200	44.461	88.514	58.257	36.308	-481.937	-363.604	66.218
1300	45.178	92.101	60.724	40.790	-480.955	-353.785	59.474
1400	45.882	95.475	63.087	45.343	-479.932	-344.041	53.705
1500	46.577	98.664	65.353	49.966	-478.870	-334.370	48.715
1600	47.265	101.692	67.531	54.658	-477.769	-324.774	44.360
1700	47.947	104.578	69.626	59.419	-476.627	-315.247	40.526
1800	48.625	107.338	71.645	64.247	-475.452	-305.787	37.126
1900	49.300	109.985	73.593	69.144	-474.236	-296.394	34.091
2000	49.972	112.531	75.477	74.107	-472.993	-287.064	31.367
2100	50.642	114.985	77.300	79.138	-471.719	-277.800	28.910
2150	50.976	116.181	78.191	81.678	-471.070	-273.193	27.769
2150	56.000	132.981	78.191	117.798	-434.950	-273.193	27.769
2200	56.000	134.268	79.450	120.598	-434.052	-269.434	26.764
2300	56.000	136.757	81.888	126.198	-432.290	-261.992	24.894
2400	56.000	139.141	84.225	131.798	-430.575	-254.632	23.186
2500	56.000	141.427	86.467	137.398	-428.923	-247.334	21.621
2600	56.000	143.623	88.624	142.998	-427.319	-240.100	20.181
2700	56.000	145.736	90.700	148.598	-425.798	-232.928	18.853
2800	56.000	147.773	92.702	154.198	-424.367	-225.814	17.625
2900	56.000	149.738	94.635	159.798	-423.053	-218.743	16.484
3000	56.000	151.637	96.504	165.398	-421.873	-211.724	15.423
3100	56.000	153.473	98.312	170.998	-420.844	-204.726	14.432
3200	56.000	155.251	100.064	176.598	-419.981	-197.777	13.507
3270	56.000	156.463	101.258	180.518	-419.476	-192.917	12.893
3270	56.000	156.463	101.258	180.518	-432.878	- 92.917	12.893
3300	56.000	156.974	101.762	182.198	-432.433	-190.717	12.630
3400	56.000	158.646	103.411	187.798	-430.958	-183.419	11.789
3500	56.000	160.269	105.012	193.398	-429.493	-176.148	10.999
3600	56.000	161.847	106.569	198.998	-428.038	-168.935	10.255
3700	56.000	163.381	108.084	204.598	-426.591	-161.761	9.554
3800	56.000	164.874	109.559	210.198	-425.153	-154.617	8.892
3900	56.000	166.329	110.996	215.798	-423.726	-147.518	8.266
4000	56.000	167.747	112.397	221.398	-422.306	-140.450	7.673
4100	56.000	169.130	113.764	226.998	-420.896	-133.427	7.112
4200	56.000	170.479	115.098	232.598	-419.496	-126.421	6.578
4300	56.000	171.797	116.402	238.198	-418.103	-119.459	6.071
4400	56.000	173.084	117.675	243.798	-416.723	-112.526	5.589
4500	56.000	174.343	118.921	249.398	-415.351	-105.638	5.130
4600	56.000	175.573	120.139	254.998	-413.991	-98.753	4.692
4700	56.000	176.778	121.331	260.598	-412.643	-91.912	4.274
4800	56.000	177.957	122.499	[illegible]	-411.311	-85.099	3.874
4900	56.000	179.111	123.642	271.198	-409.993	-78.318	3.493
5000	56.000	180.243	124.763	277.398	-408.696	-71.560	3.128
5100	56.000	181.352	125.862	282.998	-407.421	-64.824	2.778
5200	56.000	182.439	126.939	288.598	-406.171	-58.114	2.442
5300	56.000	183.506	127.997	294.198	-404.953	-51.437	2.121
5400	56.000	184.553	129.034	299.798	-403.773	-44.766	1.812
5500	56.000	185.580	130.053	305.398	-402.636	-38.115	1.514
5600	56.000	166.589	131.054	310.998	-401.553	-31.496	1.229
5700	56.000	187.580	132.037	316.598	-400.533	-24.891	0.954
5706.65	56.000	187.646	132.102	316.971	-400.467	-24.450	0.936
5706.65	56.000	187.646	132.102	316.971	-762.913	-24.450	0.936
5800	56.000	188.554	133.003	322.198	-762.345	-12.366	0.466
5900	56.000	189.512	133.953	327.798	-761.834	0.563	-0.021
6000	56.000	190.453	134.886	333.398	-761.438	13.512	-0.492

15 September 1963 HLS

TANTALUM PENTOXIDE (Ta_2O_5) (CONDENSED PHASE) gfw = 441.90

$\Delta H^{\circ}_{f298.15}$ = -488.7 ± 0.4 kcal. gfw^{-1} $S^{\circ}_{298.15}$ = 34.2 ± 0.3 cal degK^{-1}gfw^{-1}

T_m = 2150 °K ΔH_m = 36.12 kcal gfw^{-1}

$H^{\circ}_{298.15} - H^{\circ}_0$ = 5.495 kcal gfw^{-1}

$C^{\circ}_p = 37.0 + 6.56 \times 10^{-3}\,T - 5.92 \times 10^5\,T^{-2}$ cal deg K^{-1} gfw^{-1} 298.15°K ≤ T ≤ 2150°K

C°_p = 56 cal deg K^{-1} gfw^{-1} 2150 °K ≤ T ≤ 6000°K

Structure

Structure is in doubt. Often orthorhombic structure is quoted.

Heat of Formation

Based on average of Humphrey[1] and Huber et al.[2]

Heat Capacity and Entropy

Low temperature data is from Kelley.[3] High temperature data from Orr[4] is extrapolated to melting point. Data above melting point is estimated.

Melting and Vaporization

Heat of fusion is estimated.

References

1. Humphrey, G. L., J. Am. Chem. Soc. 76, 978 (1954)
2. Huber, E. J., Jr., et al, J. Phys. Chem 67, 793 (1963)
3. Kelley, K. K., J. Am. Chem. Soc. 62 818 (1940)
4. Orr, R. L., J. Am. Chem. Soc. 75, 2808 (1953)

TANTALUM PENTOXIDE (Ta_2O_5) (CONDENSED PHASE) GFW = 441.90

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^{\circ}_T - H^{\circ}_{298})/T$ (cal/°K gfw)	$H^{\circ}_T - H^{\circ}_{298}$ (Kcal/gfw)	ΔH°_f (Kcal/gfw)	ΔF°_f (Kcal/gfw)	Log K_p
298.15	±1.000	±0.300	±0.300	±0.000	±0.400		
1000	±1.000	±1.510	±0.808	±0.702			
2000	±1.000	±2.203	±1.352	±1.702			
2150	±1.000	±2.276	±1.414	±1.852			
2150	±4.000	±4.601	±1.414	±6.852			
3000	±4.000	±5.934	±2.517	±10.252			
4000	±4.000	±7.085	±3.522	±14.252			
5000	±4.000	±7.977	±4.327	±18.252			
6000	±4.000	±8.706	±4.998	±22.252			

TABLE 217

TRITITANIUM PENTOXIDE   CONDENSED PHASE O_5Ti_3

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ti from 0° to 1950°K, Liquid Ti from 1950° to 3550°K, Gaseous Ti from 3550° to 6000°K; Gaseous O_2. Solid Ti_3O_5 from 0° to 2173°K, Liquid Ti_3O_5 from 2173° to 6000°K

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-5.510	-584.523	-584.523	INFINITE
298.15	44.265	30.900	30.900	0.000	-587.650	-553.778	405.911
300	44.320	31.174	30.901	0.082	-587.633	-553.568	403.255
400	47.270	44.328	32.674	4.661	-586.689	-542.352	296.313
450	48.745	49.981	34.288	7.062	-586.159	-536.878	260.731
450	45.200	54.959	34.288	9.302	-583.919	-536.878	260.731
500	45.600	59.742	36.598	11.572	-583.553	-531.629	232.364
600	46.400	68.126	41.173	16.172	-582.862	-521.309	189.878
700	47.200	75.339	45.551	20.852	-582.206	-511.104	159.566
800	48.000	81.694	49.679	25.612	-581.571	-500.990	136.858
900	48.800	87.394	53.558	30.452	-580.941	-490.954	119.214
1000	49.600	92.577	57.205	35.372	-580.311	-480.987	105.115
1100	50.400	97.341	60.640	40.372	-579.671	-471.088	93.592
1155	50.840	99.811	62.447	43.156	-579.309	-465.666	88.109
1155	50.840	99.811	62.447	43.156	-582.159	-465.666	88.109
1200	51.200	101.761	63.885	45.452	-581.859	-461.132	83.980
1300	52.000	105.891	66.959	50.612	-581.175	-451.104	75.834
1400	52.800	109.774	69.880	55.852	-580.465	-441.123	68.859
1500	53.600	113.444	72.663	61.172	-579.770	-431.198	62.822
1600	54.400	116.929	75.321	66.572	-578.946	-421.321	57.547
1700	55.200	120.251	77.867	72.052	-578.136	-411.493	52.898
1800	56.000	123.428	80.311	77.612	-577.292	-401.716	48.773
1900	56.800	126.478	82.661	83.252	-576.410	-391.983	45.086
1950	57.200	127.958	83.803	86.102	-575.954	-387.132	43.387
1950	57.200	127.958	83.803	86.102	-587.054	-387.132	43.387
2000	57.600	129.411	84.926	88.972	-586.515	-382.016	41.743
2100	58.400	132.241	87.112	94.772	-585.380	-371.819	38.694
2173	58.984	134.247	88.662	99.056	-584.510	-364.412	36.649
2173	60.000	157.256	88.662	14[illegible].056	-534.510	-364.412	36.649
2200	60.000	157.997	89.508	150.676	-534.153	-362.299	35.989
2300	60.000	160.664	92.544	156.676	-532.843	-354.519	33.685
2400	60.000	163.218	95.436	162.676	-531.548	-346.790	31.578
2500	60.000	165.667	98.197	168.676	-530.268	-339.124	29.645
2600	60.000	168.020	100.837	174.676	-528.998	-331.494	27.863
2700	60.000	170.285	103.368	180.676	-527.743	-323.929	26.219
2800	60.000	172.467	105.797	186.676	-526.493	-316.397	24.695
2900	60.000	174.572	108.132	192.676	-525.[illegible]	-308.915	23.279
3000	60.000	176.607	110.381	198.676	-524.04[illegible]	-301.478	21.962
3100	60.000	178.574	112.549	204.676	-522.841	-294.075	20.731
3200	60.000	180.479	114.642	210.676	-521.646	-286.720	19.581
3300	60.000	182.326	116.666	216.676	-520.[illegible]58	-279.390	18.502
3400	60.000	184.116	118.623	222.676	-519.283	-272.101	17.490
3500	60.000	185.856	120.519	228.676	-518.118	-264.847	16.537
3550	60.000	186.707	121.446	231.676	-517.538	-261.238	16.082
3550	60.000	186.707	121.446	231.676	-824.909	-261.238	16.082
3600	60.000	187.546	122.358	234.676	-824.349	-253.302	15.377
3700	60.000	189.190	124.142	240.676	-823.262	-237.452	14.025
3800	60.000	190.790	125.875	246.676	-822.226	-221.628	12.746
3900	60.000	192.348	127.560	252.676	-821.243	-205.846	11.535
4000	60.000	193.867	129.198	258.676	-820.303	-190.068	10.384
4100	60.000	195.349	130.794	264.676	-819.412	-174.325	9.292
4200	60.000	196.795	132.348	270.676	-818.567	-15[illegible].595	8.252
4300	60.000	198.207	133.863	276.676	-817.765	-14[illegible].984	7.262
4400	60.000	199.586	135.341	[illegible].676	-817.009	-127.194	6.317
4500	60.000	200.934	136.784	268.675	-816.294	-111.541	5.417
4600	60.000	202.253	138.193	294.676	-815.621	-95.869	4.555
4700	60.000	203.544	139.570	300.676	-814.993	-80.238	3.731
4800	60.000	204.807	140.916	306.676	-814.408	-64.601	2.941
4900	60.000	206.044	142.232	312.676	-813.864	-48.976	2.184
5000	60.000	207.256	143.521	318.676	-813.365	-33.375	1.459
5100	60.000	208.444	144.782	324.676	-812.915	-17.776	0.762
5200	60.000	[illegible]09.609	146.018	330.676	-812.511	-2.192	0.092
5300	60.000	210.752	147.228	336.676	-812.160	13.404	-0.553
5400	60.000	211.874	148.415	342.676	-811.868	28.971	-1.172
5500	60.000	212.975	149.579	348.676	-811.637	44.561	-1.771
5600	60.000	214.056	150.721	354.676	-811.478	60.116	-2.346
5700	60.000	215.118	151.841	360.676	-811.397	75.705	-2.903
5800	60.000	216.161	152.941	366.676	-811.411	91.278	-3.439
5900	60.000	217.187	154.021	372.676	-811.530	106.863	-3.958
6000	60.000	218.195	155.083	378.676	-811.770	122.438	-4.460

31 December 1963   HLS

TRITITANIUM PENTOXIDE (Ti_3O_5) (CONDENSED PHASE) gfw = 223.70

$\Delta H^o_{f298.15}$ = -587.65 kcal gfw^{-1}

$S^o_{298.15}$ = 30.9 cal degK^{-1}gfw^{-1}

T_t = 450°K

ΔH_t = 2.240 kcal gfw^{-1}

T_m = 2173°K

ΔH_m = 50.0 kcal gfw^{-1}

$H^o_{298.15} - H^o_0$ = 5.510 kcal gfw^{-1}

C^o_p = 35.47 + 29.50x10^{-3}T cal degK^{-1}gfw^{-1} 298°K $\leq$ T $\leq$ 450°K

C^o_p = 41.60 + 8.00x10^{-3}T cal degK^{-1}gfw^{-1} 450°K $\leq$ T $\leq$ 2173°K

C^o_p = 60.0 cal degK^{-1}gfw^{-1} 2173°K $\leq$ T $\leq$ 6000°K

Structure

According to Asbrink and Magneli,[1] the low-temperature form of Ti_3O_5 is monoclinic, and the high-temperature form is of anosovite type.

Heat of Formation

Calorimetric value as compiled by Kelley and Mah[2] used.

Heat Capacity and Entropy

Low-temperature data by Shomate.[3] High-temperature data by Naylor[4] to 1600°K extrapolated to melting point. Data at higher temperatures estimated.

Melting and Vaporization

Heat of fusion estimated.

References

1. Asbrink, S. and A. Magneli, Acta Cryst. 12, 575 (1959).
2. Kelley, K. and A. Mah, U.S. Bur. Mines, Rept. 5490 (1959).
3. Shomate, C.,J. Am. Chem. Soc. 68, 310 (1946).
4. Naylor, B., J. Am. Chem. Soc. 68, 1077 (1946).

TRITITANIUM PENTOXIDE (Ti_3O_5) (CONDENSED PHASE) GFW = 223.70

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw C^o_p	S^o_T	$-(F^o_T - H^o_{298})/T$	Kcal/gfw $H^o_T - H^o_{298}$	ΔH^o_f	ΔF^o_f	Log K_p
298.15	± 1.000	± 0.200	± 0.200	± 0.000	± 2.000		
450	± 1.000	± 0.612	± 0.274	± 0.152			
450	± 2.000	± 1.278	± 0.274	± 0.452			
1000	± 2.000	± 2.875	± 1.323	± 1.552			
2000	± 2.000	± 4.262	± 2.486	± 3.552			
2173	± 2.000	± 4.428	± 2.634	± 3.898			
2173	± 5.000	± 9.029	± 2.634	± 13.898			
3000	± 5.000	±10.642	± 4.631	± 18.033			
4000	± 5.000	±12.080	± 6.322	± 23.033			
5000	± 5.000	±13.196	± 7.590	± 28.033			
6000	± 5.000	±14.108	± 8.602	± 33.033			

RHENIUM HEPTOXIDE

TABLE 218

CONDENSED PHASE

O_7Re_2

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Re from 0° to 3453°K, Liquid Re from 3453° to 5961°K, Gaseous Re from 5961° to 6000°K, Gaseous O_2, Solid Re_2O_7 from 0° to 570°K, Liquid Re_2O_7 from 570° to 634°K.

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-7.246	-294.070	-294.070	INFINITE
298.15	39.737	49.543	49.543	0.000	-296.700	-255.032	186.935
300	39.850	49.789	49.544	0.074	-296.693	-254.774	185.594
400	45.344	62.028	51.175	4.341	-296.155	-240.869	131.598
500	50.250	72.680	54.432	9.124	-295.193	-227.150	99.285
570	53.537	79.475	57.095	12.757	-294.300	-217.696	83.465
570	71.100	105.791	57.095	27.757	-279.300	-217.696	83.465
600	71.100	109.438	59.622	29.890	-278.557	-214.463	78.114
634	71.100	113.357	62.400	32.307	-277.299	-210.878	72.689

RHENIUM HEPTOXIDE (Re_2O_7) (CONDENSED PHASE) gfw = 484.44

$\Delta H^\circ_{f298.15}$ = -296.7 kcal gfw^{-1}

$S^\circ_{298.15}$ = 49.54 cal deg K^{-1} gfw^{-1}

T_m = 570°K

ΔH_m = 15.0 kcal gfw^{-1}

T_b = 634°K

ΔH_v = 17.3 kcal gfw^{-1}

$H^\circ_{298.15} - H^\circ_0$ = 7.246 kcal gfw^{-1}

$C^\circ_p = 29.15 + 4.4 \times 10^{-2}\,T - 2.25 \times 10^5\,T^{-2}$ cal deg K^{-1} gfw^{-1} 298.15°K $\leq T \leq$ 570°K

C°_p = 71.10 cal deg K^{-1} gfw^{-1} (estimated) 570°K $\leq T \leq$ 634°K

Structure

Preliminary investigations of crystal structure indicate an orthorhombic type.[1]

Heat of Formation

Heat of formation has been determined by Roth and Becker,[2] and by Boyd *et al.*[3] The average of these two determinations has been adopted here.

Heat Capacity and Entropy

Entropy at 298°K has been calculated from low-temperature heat-capacity data of Busey.[4] Heat capacity of solid has been extrapolated to melting point. Heat capacity of liquid is estimated.

Melting and Vaporization

Melting and boiling temperatures have been calculated from vapor-pressure data of Ogawa[5] and Smith *et al.*[6]

References

1. Wilhelmi, V., Acta Chem. Scand. 8, 693 (1954).
2. Roth, W. A. and G. Becker, Z. Physik Chem. 159, 27 (1932).
3. Boyd, G. E., J. W. Cobble, and W. T. Smith, Jr., J. Am. Chem. Soc. 75, 5773 (1953).
4. Busey, R. H., J. Am. Chem. Soc. 78, 3263 (1956).
5. Ogawa, E., Bull. Chem. Soc. Japan 7, 265 (1932).
6. Smith, W. T., L. E. Line, and W. A. Bell, J. Am. Chem. Soc. 74, 4964 (1952).

RHENIUM HEPTOXIDE (Re_2O_7) (CONDENSED PHASE) GFW = 484.44

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal/gfw)	ΔH°_f (Kcal/gfw)	ΔF°_f (Kcal/gfw)	Log K_p
298.15	± 0.040	± 0.050	± 0.050	± 0.000	± 2.000		
300	± 0.040	± 0.050	± 0.050	± 0.000			
400	± 0.040	± 0.062	± 0.052	± 0.004			
500	± 0.040	± 0.071	± 0.055	± 0.008			
570	± 0.040	± 0.076	± 0.057	± 0.011			
570	± 1.000	± 0.953	± 0.057	± 0.511			
600	± 1.000	± 1.004	± 0.103	± 0.541			
634	± 1.000	± 1.060	± 0.153	± 0.575			

TABLE 219

OSMIUM

REFERENCE STATE

Os

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Os from 0° to 3290°K, Liquid Os from 3290° to 5270°K, Gaseous from 5270° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.210			
298.15	5.952	7.800	7.800	0.000			
300	5.954	7.837	7.801	0.011			
400	6.042	9.562	8.035	0.611			
500	6.130	10.919	8.481	1.219			
600	6.218	12.045	8.983	1.837			
700	6.306	13.010	9.491	2.463			
800	6.394	13.858	9.985	3.098			
900	6.482	14.616	10.458	3.742			
1000	6.570	15.303	10.909	4.394			
1100	6.658	15.934	11.338	5.056			
1200	6.746	16.517	11.745	5.726			
1300	6.834	17.060	12.133	6.405			
1400	6.922	17.570	12.504	7.093			
1500	7.010	18.051	12.858	7.789			
1600	7.098	18.506	13.196	8.495			
1700	7.186	18.939	13.522	9.209			
1800	7.274	19.352	13.834	9.932			
1900	7.362	19.748	14.135	10.664			
2000	7.450	20.127	14.425	11.404			
2100	7.538	20.493	14.706	12.154			
2200	7.626	20.846	14.977	12.912			
2300	7.714	21.187	15.239	13.679			
2400	7.802	21.517	15.494	14.455			
2500	7.890	21.837	15.741	15.239			
2600	7.978	22.148	15.982	16.033			
2700	8.066	22.451	16.216	16.835			
2800	8.154	22.746	16.444	17.646			
2900	8.242	23.034	16.666	18.466			
3000	8.330	23.315	16.883	19.294			
3100	8.418	23.589	17.095	20.132			
3200	8.506	23.858	17.302	20.978			
3290	8.585	24.095	17.485	21.747			
3290	9.000	26.395	17.485	29.314			
3300	9.000	26.422	17.512	29.404			
3400	9.000	26.691	17.778	30.304			
3500	9.000	26.952	18.036	31.204			
3600	9.000	27.205	18.287	32.104			
3700	9.000	27.452	18.532	33.004			
3800	9.000	27.692	18.770	33.904			
3900	9.000	27.926	19.001	34.804			
4000	9.000	28.153	19.227	35.704			
4100	9.000	28.376	19.448	36.604			
4200	9.000	28.593	19.663	37.504			
4300	9.000	28.804	19.873	38.404			
4400	9.000	29.011	20.078	39.304			
4500	9.000	29.213	20.279	40.204			
4600	9.000	29.411	20.476	41.104			
4700	9.000	29.605	20.668	42.004			
4800	9.000	29.794	20.856	42.904			
4900	9.000	29.980	21.040	43.804			
5000	9.000	30.162	21.221	44.704			
5100	9.000	30.340	21.398	45.604			
5200	9.000	30.515	21.572	46.504			
5269.57	9.000	30.634	21.690	47.130			
5269.57	8.769	64.110	21.690	223.531			
5300	8.773	64.161	21.935	223.798			
5400	8.809	64.326	22.719	224.677			
5500	8.838	64.488	23.447	225.560			
5600	8.866	64.647	24.210	226.445			
5700	8.893	64.804	24.921	227.333			
5800	8.919	64.959	25.610	228.224			
5900	8.944	65.112	26.279	229.117			
6000	8.968	65.262	26.927	230.012			

15 September 1962 RCF

OSMIUM (Os) (REFERENCE STATE) gfw = 190.2

$0^{\circ}K$ to $3290^{\circ}K$	Crystal
$3290^{\circ}K$ to $5269.57^{\circ}K$	Liquid
$5269.57^{\circ}K$ to $6000^{\circ}K$	Ideal Monatomic Gas

ΔH^{o}_{f0} = 0 kcal gfw^{-1} $\Delta H^{o}_{f298.15}$ = 0 kcal gfw^{-1}

$\Delta H^{o}_{s298.15}$ = 187.400 kcal gfw^{-1} $S^{o}_{298.15}$ = 7.800 cal deg K^{-1}gfw^{-1}

T_m = 3290°K H_m = 7.567 kcal gfw^{-1}

T_b = 5269.57°K H_v = 176.401 kcal gfw^{-1}

$H^{o}_{298.15}-H^{o}_{0}$ = 1.210 kcal gfw^{-1}

C^{o}_{p} = 5.690 + 0.880 x 10^{-3}T cal deg K^{-1}gfw^{-1} 298.15°K $\leq$ T $\leq$ 3290°K

C^{o}_{p} = 9.000 cal deg K^{-1}gfw^{-1} 3290°K $\leq$ T $\leq$ 5269.57°K

Structure

An hcp (A3) type. See volume 1, this study (section IVA18) for details.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Kelley's[1] equation used in compilation and extrapolated to melting point.

Melting

See volume 1, this study (section IVA18) for details.

Vaporization

Data from Panish and Reif.[2]

References

1. Kelley, K. K., U. S. Bur. Mines, Bull. 584 (1960).
2. Panish, M. B. and L. Reif, J. Chem. Phys. 37, 128 (1962).

OSMIUM (Os) (REFERENCE STATE) GFW = 190.2

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_{p} (cal/°K gfw)	S°_{T} (cal/°K gfw)	$-(F^{\circ}_{T} - H^{\circ}_{298})/T$ (cal/°K gfw)	$H^{\circ}_{T} - H^{\circ}_{298}$ (Kcal/gfw)	ΔH°_{f} (Kcal/gfw)	ΔF°_{f} (Kcal/gfw)	Log K_p
298.15	±0.100	±0.500	±0.500	±0.000			
1000	±0.500	±0.740	±0.600	±0.140			
2000	±1.000	±1.260	±0.810	±0.890			
3000	±1.500	±1.770	±0.890	±2.140			
3290	±1.640	±1.910	±1.120	±2.580			
3290	±0.450	±2.270	±1.120	±3.780			
4000	±1.750	±2.490	±1.350	±4.570			
5000	±3.350	±3.080	±1.640	±7.220			
5269.57	±4.050	±3.230	±1.660	±8.290			
5269.57	±0.008	±0.010	±0.005	±0.029			
6000	±0.004	±0.001	±0.006	±0.034			

TABLE 220

OSMIUM

IDEAL MONATOMIC GAS **Os**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Os from 0° to 3290°K, Liquid Os from 3290° to 5270°K, Gaseous Os from 5270° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.481	187.129	187.129	INFINITE
298.15	4.968	46.002	46.002	0.000	187.400	176.010	-129.013
300	4.969	46.032	46.002	0.009	187.398	175.940	-128.460
400	4.974	47.462	46.197	0.506	187.295	172.135	-94.046
500	4.996	48.574	46.565	1.005	187.186	168.358	-73.586
600	5.044	49.489	46.978	1.506	187.069	164.603	-59.954
700	5.122	50.272	47.394	2.014	186.951	160.868	-50.223
800	5.231	50.962	47.798	2.532	186.834	157.150	-42.929
900	5.367	51.586	48.185	3.061	186.719	153.446	-37.260
1000	5.522	52.159	48.554	3.606	186.612	149.755	-32.727
1100	5.691	52.694	48.906	4.166	186.510	146.075	-29.021
1200	5.867	53.196	49.243	4.744	186.418	142.403	-25.934
1300	6.042	53.673	49.565	5.340	186.335	138.738	-23.323
1400	6.211	54.127	49.875	5.952	186.259	135.081	-21.086
1500	6.372	54.561	50.173	6.582	186.193	131.428	-19.148
1600	6.521	[illegible].977	50.460	7.226	186.131	127.778	-17.453
1700	6.658	[illegible].376	50.738	7.885	186.076	124.133	-15.958
1800	6.782	55.761	51.006	8.557	18[illegible].025	120.490	-14.629
1900	6.894	56.130	51.266	9.241	185.977	116.851	-13.440
2000	6.996	56.486	51.519	9.936	185.932	113.212	-12.371
2100	7.088	56.830	51.763	10.640	185.887	109.580	-11.404
2200	7.173	57.162	52.001	11.353	185.841	105.948	-10.524
2300	7.251	57.482	52.233	12.074	185.795	102.314	-9.722
2400	7.324	57.793	52.458	12.803	185.748	98.686	-8.986
2500	7.393	58.093	52.677	13.539	185.700	95.060	-8.310
2600	7.459	58.384	52.891	14.282	185.649	91.437	-7.686
2700	7.523	58.667	53.100	15.031	185.596	87.813	-7.108
2800	7.584	58.942	53.304	15.786	185.540	84.192	-6.571
2900	7.645	59.209	53.503	16.548	185.482	80.573	-6.072
3000	7.704	59.469	53.697	17.315	185.421	76.958	-5.606
3100	7.763	59.722	53.888	18.088	185.356	73.342	-5.170
3200	7.821	59.970	54.074	18.868	185.290	69.730	-4.762
3290	7.872	60.188	54.238	19.574	185.227	66.483	-4.416
3290	7.872	60.188	54.238	19.574	177.660	66.483	-4.416
3300	7.878	60.211	54.256	19.653	177.649	66.145	-4.380
3400	7.934	60.447	54.435	20.443	177.539	62.766	-4.034
3500	7.990	60.678	54.610	21.239	[illegible]	59.391	-3.708
3600	8.045	60.904	54.782	22.041	177.[illegible]	56.018	-3.401
3700	8.098	61.125	54.950	22.848	177.244	52.653	-3.110
3800	8.151	61.342	55.115	23.661	177.157	49.289	-2.835
3900	8.203	61.554	55.278	24.478	177.074	45.920	-2.573
4000	8.253	61.763	55.437	25.301	176.997	42.560	-2.325
4100	8.302	61.967	55.594	26.129	176.925	39.201	-2.090
4200	8.350	62.168	55.748	26.962	176.858	35.843	-1.865
4300	8.396	62.365	55.900	27.799	176.795	32.484	-1.651
4400	8.441	62.558	56.049	28.641	176.737	29.128	-1.447
4500	8.484	62.748	56.196	29.487	176.683	25.773	-1.252
4600	8.526	62.935	56.340	30.338	176.634	22.426	-1.065
4700	8.567	63.119	56.482	31.192	176.588	19.074	-0.887
4800	8.605	[illegible].300	56.623	32.051	176.547	15.718	-0.716
4900	8.643	63.478	56.761	32.913	176.509	12.367	-0.552
5000	8.679	63.653	56.897	33.779	176.475	9.020	-0.394
5100	8.713	63.825	57.031	34.649	176.445	5.672	-0.243
5200	8.746	63.994	57.163	35.522	176.418	2.327	-0.098
5269.57	8.769	64.110	57.254	36.131	176.401	0.000	0.000
5269.57	8.769	64.110	57.254	36.131			
5300	8.773	64.161	57.294	36.398			
5400	8.809	64.326	57.422	37.277			
5500	8.838	64.488	57.549	38.160			
5600	8.866	64.647	57.675	39.045			
5700	8.893	64.804	57.798	39.933			
5800	8.919	64.959	57.921	40.824			
5900	8.944	65.112	58.041	41.717			
6000	8.968	65.262	58.160	42.612			

15 September 1962 RCF

ΔH^o_{f0} = 187.129 kcal gfw^{-1} $\Delta H^o_{f298.15}$ = 187.400 kcal gfw^{-1}

Ground State Configuration = $^5D_4$ $S^o_{298.15}$ = 46.002 cal deg K^{-1}gfw^{-1}

$H^o_{298.15}-H^o_0$ = 1.481 kcal gfw^{-1}

Electronic Levels and Multiplicities

Energy levels from Van Kleef.[1,2]

Heat of Formation

Data from Panish and Reif.[3]

Heat Capacity and Entropy

Calculated from monatomic gas-computer program.

References

1. Van Kleef, T., Koninkl. Ned. Akad. Wetenschap. Proc. B63, 549 (1960).
2. Van Kleef, T. and P. Klinkenberg, Physica 27, 83 (1961).
3. Panish, M. B. and L. Reif, J. Chem. Phys. 37, 128 (1962).

OSMIUM, MONATOMIC (Os) (IDEAL GAS) GFW = 190.2

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T (cal/°K gfw)	$-(F^o_T - H^o_{298})/T$ (cal/°K gfw)	$H^o_T - H^o_{298}$ (Kcal/gfw)	ΔH^o_f (Kcal/gfw)	ΔF^o_f (Kcal/gfw)	Log K_p
298.15	±0.000	±0.002	±0.002	±0.000	±1.500	± 1.650	±0.840
1000	±0.000	±0.002	±0.003	±0.000	±1.640	± 2.100	±0.380
2000	±0.002	±0.003	±0.003	±0.001	±2.390	± 3.120	±0.290
3000	±0.008	±0.004	±0.003	±0.005	±3.640	± 4.170	±0.270
3290	±0.009	±0.005	±0.003	±0.008	±4.090	± 5.180	±0.310
3290	±0.009	±0.005	±0.003	±0.008	±5.290	± 5.180	±0.310
4000	±0.013	±0.007	±0.004	±0.016	±6.090	± 6.900	±0.350
5000	±0.010	±0.010	±0.002	±0.027	±8.750	± 9.700	±0.400
5269.57	±0.008	±0.010	±0.005	±0.029	±9.820	±10.250	±0.410
5269.57	±0.008	±0.010	±0.005	±0.029			
6000	±0.004	±0.011	±0.006	±0.034			

PLATINUM

REFERENCE STATE

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Pt from 0° to 2043°K, Liquid Pt from 2043° to 4108°K, Gaseous Pt from 4108° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.372			
298.15	6.180	9.950	9.950	0.000			
300	6.183	9.988	9.950	0.011			
400	6.339	11.790	10.195	0.638			
500	6.464	13.218	10.661	1.278			
600	6.583	14.407	11.189	1.931			
700	6.704	15.431	11.724	2.595			
800	6.827	16.334	12.245	3.271			
900	6.951	17.145	12.745	3.960			
1000	7.076	17.884	13.222	4.662			
1100	7.201	18.564	13.677	5.376			
1200	7.326	19.196	14.111	6.102			
1300	7.452	19.788	14.525	6.841			
1400	7.577	20.344	14.921	7.592			
1500	7.703	20.871	15.301	8.356			
1600	7.828	21.373	15.665	9.133			
1700	7.954	21.851	16.014	9.922			
1800	8.080	22.309	16.352	10.724			
1900	8.206	22.749	16.677	11.538			
2000	8.332	23.173	16.991	12.365			
2043	8.386	23.351	17.149	12.724			
2043	8.500	25.651	17.149	17.423			
2100	8.500	25.885	17.358	17.908			
2200	8.500	26.281	17.754	18.758			
2300	8.500	26.658	18.133	19.608			
2400	8.500	27.020	18.496	20.458			
2500	8.500	27.367	18.844	21.308			
2600	8.500	27.701	19.178	22.158			
2700	8.500	28.021	19.500	23.009			
2800	8.500	28.331	19.810	23.858			
2900	8.500	28.629	20.109	24.708			
3000	8.500	28.917	20.398	25.558			
3100	8.500	29.196	20.677	26.408			
3200	8.500	29.466	20.948	27.258			
3300	8.500	29.727	21.210	28.108			
3400	8.500	29.981	21.464	28.958			
3500	8.500	30.227	21.711	29.808			
3600	8.500	30.467	21.951	30.658			
3700	8.500	30.700	22.184	31.508			
3800	8.500	30.926	22.411	32.358			
3900	8.500	31.147	22.632	33.208			
4000	8.500	31.362	22.848	34.058			
4100	8.500	31.572	23.058	34.908			
4108.34	8.500	31.589	23.126	34.979			
4108.34	5.829	61.168	23.126	156.498			
4200	5.850	61.297	23.908	157.032			
4300	5.873	61.435	24.779	157.619			
4400	5.895	61.570	25.614	158.207			
4500	5.917	61.703	26.415	158.798			
4600	5.939	61.833	27.183	159.390			
4700	5.960	61.961	27.922	159.985			
4800	5.982	62.087	28.632	160.583			
4900	6.003	62.210	29.316	161.182			
5000	6.024	62.332	29.975	161.783			
5100	6.046	62.451	30.610	162.387			
5200	6.067	62.569	31.224	162.992			
5300	6.089	62.685	31.817	163.600			
5400	6.111	62.799	32.390	164.210			
5500	6.133	62.911	32.943	164.822			
5600	6.155	63.022	33.480	165.437			
5700	6.178	63.131	33.999	166.053			
5800	6.202	63.239	34.502	166.672			
5900	6.225	63.345	34.990	167.294			
6000	6.250	63.450	35.464	167.917			

15 December 1962 RCF

$0^{o}K$ to $2043^{o}K$	Crystal
$2043^{o}K$ to $4108^{o}K$	Liquid
$4108^{o}K$ to $6000^{o}K$	Ideal Monatomic Gas

$\Delta H^{o}_{f0} = 0$

$\Delta H^{o}_{f298.15} = 0$

$\Delta H^{o}_{s298.15} = 135.100$ kcal gfw^{-1}

$S^{o}_{298.15} = 9.950$ cal deg K^{-1}gfw^{-1}

$T_m = 2043^{o}K$

$\Delta H_m = 4.699$ kcal gfw^{-1}

$T_b = 4108^{o}K$

$\Delta H_v = 121.519$ kcal gfw^{-1}

$H^{o}_{298.15}-H^{o}_{0} = 1.372$ kcal gfw^{-1}

$C^{o}_{p} = 6.028 + 0.969 \times 10^{-3}T - 0.1220 \times 10^{5}T^{-2}$ cal deg K^{-1}gfw^{-1} $\quad 298.15^{o}K \leq T \leq 500^{o}K$

$C^{o}_{p} = 5.810 + 1.260 \times 10^{-3}T - 0.060 \times 10^{5}T^{-2}$ cal deg K^{-1}gfw^{-1} $\quad 500^{o}K \leq T \leq 2043^{o}K$

$C^{o}_{p} = 8.500$ cal deg K^{-1}gfw^{-1} $\quad 2043^{o}K \leq T \leq 4108^{o}K$

Structure

An f.c.c. (A1) type.

Hea of Formation

Zero by definition.

Heat Capacity and Entropy

Kelley et al[1] calculated S_{298} and that value adopted. Heat-capacity data based on measurements of several authors. Liquid heat capacity estimated.

Melting and Vaporization

Heat of fusion estimated. Melting point estimated from works of several authors. Heat of vaporization calculated. See volume 1, this study (section IVA20) for details.

Reference

1. Kelley, K. K. and E. G. King, U. S. Bur. Mines, Bull. 592 (1961).

PLATINUM (Pt) (REFERENCE STATE) GFW = 195.09

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^{o}_{p} (cal/°K gfw)	S^{o}_{T} (cal/°K gfw)	$-(F^{o}_{T} - H^{o}_{298})/T$ (cal/°K gfw)	$H^{o}_{T} - H^{o}_{298}$ (Kcal/gfw)	ΔH^{o}_{f} (Kcal/gfw)	ΔF^{o}_{f} (Kcal/gfw)	Log K_p
298.15	±0.020	±0.050	±0.050	±0.000			
1000	±0.020	±0.070	±0.060	±0.010			
2043	±0.100	±0.120	±0.080	±0.080			
2043	±0.420	±0.510	±0.080	±0.880			
3000	±2.050	±0.980	±0.290	±2.060			
4000	±3.750	±1.810	±0.570	±4.960			
4108.34	±3.930	±1.910	±0.610	±5.370			
4108.34	±0.000	±0.003	±0.003	±0.001			
5000	±0.001	±0.003	±0.003	±0.001			
6000	±0.001	±0.003	±0.003	±0.002			

TABLE 222

PLATINUM

IDEAL MONATOMIC GAS

Pt

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Pt from 0° to 2043°K, Liquid Pt from 2043° to 4108°K, Gaseous Pt from 4108° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.572	134.900	134.900	INFINITE
298.15	6.102	45.962	45.962	0.000	135.100	124.363	-91.156
300	6.113	45.999	45.962	0.011	135.100	124.296	-90.545
400	6.459	47.817	46.207	0.644	135.106	120.695	-65.942
500	6.435	49.260	46.679	1.291	135.113	117.091	-51.178
600	6.260	50.419	47.209	1.926	135.095	113.488	-41.336
700	6.059	51.369	47.738	2.542	135.047	109.890	-34.308
800	5.877	52.166	48.243	3.138	134.966	106.302	-29.039
900	5.728	52.849	48.717	3.718	134.858	102.725	-24.944
1000	5.609	53.446	49.161	4.285	134.723	99.161	-21.671
1100	5.517	53.976	49.575	4.841	134.565	95.612	-18.995
1200	5.447	54.453	49.962	5.389	134.387	92.079	-16.769
1300	5.395	54.887	50.325	5.931	134.190	88.560	-14.888
1400	5.358	55.285	50.665	6.469	133.977	85.058	-13.278
1500	5.333	55.654	50.985	7.003	133.747	81.574	-11.885
1600	5.318	55.998	51.288	7.536	133.503	78.103	-10.668
1700	5.311	56.320	51.575	8.067	133.245	74.646	-9.596
1800	5.310	56.623	51.847	8.598	13[illegible].974	71.209	-8.646
1900	5.316	56.911	52.106	9.129	132.691	67.785	-7.797
2000	5.326	57.184	52.353	9.661	132.396	64.376	-7.034
2043	5.332	57.294	52.453	9.891	132.267	62.921	-6.731
2043	5.332	57.294	52.453	9.891	127.568	62.921	-6.731
2100	5.340	57.444	52.589	10.195	127.387	61.115	-6.360
2200	5.356	57.693	52.816	10.729	127.071	57.964	-5.758
2300	5.376	57.931	53.033	11.266	126.758	54.830	-5.210
2400	5.397	58.160	53.242	11.805	126.447	51.710	-4.709
2500	5.421	58.381	53.443	12.346	126.138	48.602	-4.249
2600	5.445	58.594	53.637	12.889	125.831	45.507	-3.825
2700	5.470	58.800	53.824	13.435	125.527	42.425	-3.434
2800	5.496	59.000	54.006	13.983	125.225	39.351	-3.071
2900	5.523	59.193	54.181	14.534	124.926	36.291	-2.735
3000	5.549	59.381	54.351	15.087	124.629	33.241	-2.421
3100	5.576	59.563	54.517	15.644	124.336	30.196	-2.129
3200	5.603	59.740	54.677	16.203	124.045	27.167	-1.855
3300	5.629	59.913	54.833	16.764	123.756	24.144	-1.599
3400	5.655	60.082	54.985	17.328	123.470	21.129	-1.358
3500	5.681	60.246	55.133	17.895	12[illegible].[illegible]87	18.123	-1.132
3600	5.707	60.406	55.277	18.465	122.[illegible]	15.126	-0.908
3700	5.732	60.563	55.418	19.037	122.6[illegible]9	12.134	-0.717
3800	5.756	60.716	55.555	19.611	122.353	9.153	-0.526
3900	5.780	60.866	55.690	20.188	122.080	6.174	-0.346
4000	5.804	61.013	55.821	20.767	121.809	3.208	-0.175
4100	5.827	61.156	55.949	21.349	121.541	0.247	-0.013
4108.34	5.829	61.168	55.960	21.398	121.519	0.000	0.000
4108.34	5.829	61.168	55.960	21.398			
4200	5.850	61.297	56.075	21.932			
4300	5.873	61.435	56.198	22.519			
4400	5.895	61.570	56.319	23.107			
4500	5.917	61.703	56.437	23.698			
4600	5.939	61.833	56.553	24.290			
4700	5.960	61.961	56.666	24.885			
4800	5.982	62.087	56.778	25.483			
4900	6.003	62.210	56.888	26.082			
5000	6.024	62.332	56.995	26.683			
5100	6.046	62.451	57.101	27.287			
5200	6.067	62.569	57.205	27.892			
5300	6.089	62.685	57.307	28.500			
5400	6.111	62.799	57.408	29.110			
5500	6.133	62.911	57.507	29.722			
5600	6.155	63.022	57.605	30.337			
5700	6.178	63.131	57.701	30.953			
5800	6.202	63.239	57.795	31.572			
5900	6.22[illegible]	63.345	57.888	32.194			
6000	6.250	63.450	57.980	32.817			

15 December 1962 RCF

PLATINUM (Pt) (IDEAL MONATOMIC GAS) gfw = 195.09

ΔH^{o}_{f0} = 134.900 kcal gfw^{-1}

$\Delta H^{o}_{f298.15}$ = 135.100 kcal gfw^{-1}

Ground State Configuration = $^{3}D_{3}$

$S^{o}_{298.15}$ = 45.962 cal deg K^{-1}gfw^{-1}

$H^{o}_{298.15}-H^{o}_{0}$ = 1.572 kcal gfw^{-1}

Electronic Levels and Multiplicities

Spectroscopic energy levels from Moore.[1]

Heat of Formation

Based on several reported values. See volume 1, this study (section IVA20) for details.

Heat Capacity and Entropy

Calculated on monatomic-gas computer program.

Reference

1. Moore, C., Nat. Bur. Stds. (U.S.) Circ. 467, Vol. 3 (May 1958).

PLATINUM, MONATOMIC (Pt) (IDEAL GAS) GFW = 195.09

SUMMARY OF UNCERTAINTY ESTIMATES

	cal/°K gfw			Kcal gfw			
T, °K	C^{o}_{p}	S^{o}_{T}	$-(F^{o}_{T} - H^{o}_{298})/T$	$H^{o}_{T} - H^{o}_{298}$	ΔH_f	ΔF_f	Log K_p
298.15	± 0.000	± 0.002	±0.003	± 0.000	± 0.300	± 0.320	± 0.230
1000	± 0.000	± 0.003	±0.003	± 0.000	± 0.310	± 0.360	± 0.080
2000	± 0.000	± 0.003	±0.003	± 0.000			
2043	± 0.000	± 0.003	±0.003	± 0.000	± 0.380	± 0.470	± 0.050
2043	± 0.000	± 0.003	±0.003	± 0.000	± 1.180	± 0.470	± 0.050
3000	± 0.000	± 0.003	±0.003	± 0.001	± 2.360	± 1.180	± 0.090
4000	± 0.000	± 0.003	±0.003	± 0.001	± 5.260	± 2.590	± 0.140
4108.34	± 0.000	± 0.003	±0.003	± 0.001	± 5.670	± 2.820	± 0.150
4108.34	± 0.000	± 0.003	±0.003	± 0.001			
5000	± 0.001	± 0.003	±0.003	± 0.001			
6000	± 0.001	± 0.003	±0.003	± 0.002			

TABLE 223

RHENIUM

REFERENCE STATE

Re

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Re from 0° to 3453°K, Liquid Re from 3453° to 5960°K, Gaseous Re from 5960° to 6000°K

T, °K	cal/°K gfw.			Kcal/gfw.			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.307			
298.15	6.160	8.886	8.886	0.000			
300	6.162	8.924	8.886	0.011			
400	6.262	10.710	9.129	0.633			
500	6.365	12.119	9.591	1.264			
600	6.472	13.289	10.112	1.906			
700	6.583	14.295	10.640	2.558			
800	6.697	15.181	11.153	3.222			
900	6.815	15.977	11.645	3.898			
1000	6.936	16.701	12.115	4.585			
1100	7.061	17.368	12.563	5.285			
1200	7.189	17.988	12.989	5.998			
1300	7.321	18.568	13.396	6.723			
1400	7.456	19.116	13.786	7.462			
1500	7.595	19.635	14.158	8.215			
1600	7.738	20.130	14.516	8.981			
1700	7.884	20.603	14.860	9.762			
1800	8.033	21.058	15.192	10.558			
1900	8.186	21.496	15.513	11.369			
2000	8.343	21.920	15.822	12.195			
2100	8.503	22.331	16.123	13.038			
2200	8.667	22.730	16.414	13.896			
2300	8.834	23.119	16.697	14.771			
2400	9.005	23.499	16.973	15.663			
2500	9.179	23.870	17.241	16.572			
2600	9.357	24.233	17.503	17.499			
2700	9.539	24.590	17.759	18.444			
2800	9.723	24.940	18.009	19.407			
2900	9.912	25.285	18.254	20.389			
3000	10.104	25.624	18.494	21.389			
3100	10.300	25.958	18.730	22.410			
3200	10.499	26.289	18.961	23.450			
3300	10.701	26.615	19.188	24.509			
3400	10.908	26.937	19.411	25.590			
3453	11.018	27.107	19.528	26.171			
3453	11.000	29.407	19.528	34.113			
3500	11.000	29.556	19.661	34.630			
3600	11.000	29.865	19.940	35.730			
3700	11.000	30.167	20.213	36.830			
3800	11.000	30.460	20.479	37.930			
3900	11.000	30.746	20.738	39.030			
4000	11.000	31.024	20.992	40.130			
4100	11.000	31.296	21.240	41.230			
4200	11.000	31.561	21.483	42.330			
4300	11.000	31.820	21.720	43.430			
4400	11.000	32.073	21.952	44.530			
4500	11.000	32.320	22.180	45.630			
4600	11.000	32.562	22.403	46.730			
4700	11.000	32.798	22.622	47.830			
4800	11.000	33.030	22.836	48.930			
4900	11.000	33.257	23.047	50.030			
5000	11.000	33.479	23.253	51.130			
5100	11.000	33.697	23.456	52.230			
5200	11.000	33.910	23.655	53.330			
5300	11.000	34.120	23.850	54.430			
5400	11.000	34.326	24.042	55.530			
5500	11.000	34.527	24.231	56.630			
5600	11.000	34.726	24.417	57.730			
5700	11.000	34.920	24.599	58.830			
5800	11.000	35.112	24.779	59.930			
5900	11.000	35.300	24.956	61.030			
5960.67	11.0[illegible]	35.412	25.061	61.696			
5960.67	13.1[illegible]	63.650	25.061	230.011			
6000	13.178	63.738	25.316	230.530			

0^oK to 3453^oK	Crystal
3453^oK to 5960^oK	Liquid
5960^oK to 6000^oK	Ideal Monatomic Gas

$\Delta H^o_{f0} = 0$ $\Delta H^o_{f298.15} = 0$

$\Delta H_{s298.15} = 185.370$ kcal gfw^{-1} $S^o_{298.15} = 8.886$ cal deg K^{-1}gfw^{-1}

$T_m = 3453^oK$ $\Delta H_m = 7.942$ kcal gfw^{-1}

$T_b = 5960^oK$ $\Delta H_v = 168.315$ kcal gfw^{-1}

$H^o_{298.15} - H^o_0 = 1.307$ kcal gfw^{-1}

$C^o_p = 5.883 + 0.876 \times 10^{-3}T + 0.0177 \times 10^{-5}T^2$ cal deg K^{-1}gfw^{-1}

$298.15^oK \leq T \leq 3453^oK$

$C^o_p = 11.000$ cal deg K^{-1}gfw^{-1} $3453^oK \leq T \leq 5960^oK$

Structure

An h. c. p. (A3) type.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Entropy based on Keesom et al.[1] High-temperature heat-capacity data of Jaeger et al[2] joined to low-temperature data. Liquid heat capacity estimated.

Melting and Vaporization

Heat of fusion estimated. Sims et al[3] melting point adopted. Heat of vaporization calculated and based on Sherwood et al.[4]

References

1. Keesom, P. H. and C. A. Bryant, Phys. Rev. Letters 2, 260 (1959).
2. Jaeger, F. M. and E. Rosenbohm, Proc. Acad. Sci. Amsterdam 36, 786 (1933).
3. Sims, C. T., C. M. Craighead, and R. I. Jaffee, J. Metals 7, 168 (1955).
4. Sherwood, E. M. et al, J. Electrochem. Soc. 102, 650 (1955).

RHENIUM (Re) (REFERENCE STATE) GFW = 186.22

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T	$-(F^o_T - H^o_{298})/T$	$H^o_T - H^o_{298}$ (Kcal/gfw)	ΔH^o_f	ΔF^o_f	Log K_p
298.15	±0.040	±0.050	±0.050	± 0.000			
1000	±0.100	±0.090	±0.070	± 0.020			
2000	±0.500	±0.290	±0.130	± 0.320			
3000	±1.000	±0.600	±0.240	± 1.070			
3453	±1.500	±0.770	±0.300	± 1.640			
3453	±1.550	±1.210	±0.300	± 3.140			
4000	±1.750	±1.380	±0.440	± 3.770			
5000	±3.950	±2.010	±0.690	± 6.620			
5960.67	±6.070	±2.890	±0.970	±11.430			
5960.67	±0.009	±0.005	±0.003	± 0.012			

TABLE 224

RHENIUM **Re**

IDEAL MONATOMIC GAS

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Re from 0° to 3453°K, Liquid Re from 3453° to 5960°K, Gaseous Re from 5960° to 6000°K

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.481	185.196	185.196	INFINITE
298.15	4.968	45.133	45.133	0.000	185.370	174.563	-127.952
300	4.968	45.163	45.133	0.009	185.368	174.496	-127.114
400	4.968	46.593	45.328	0.506	185.243	170.890	-93.366
500	4.968	47.701	45.696	1.003	185.109	167.318	-73.131
600	4.968	48.607	46.108	1.500	184.964	163.772	-59.651
700	4.968	49.373	46.521	1.996	184.808	160.253	-50.031
800	4.968	50.036	46.920	2.493	184.641	156.756	-42.822
900	4.968	50.622	47.299	2.990	184.462	153.281	-37.220
1000	4.968	51.145	47.658	3.487	184.272	149.827	-32.743
1100	4.968	51.619	47.997	3.984	184.069	146.393	-29.084
1200	4.969	52.051	48.317	4.481	183.853	142.976	-26.038
1300	4.971	52.449	48.620	4.978	183.634	139.579	-23.464
1400	4.974	52.817	48.907	5.475	183.383	136.201	-21.261
1500	4.979	53.160	49.179	5.972	183.127	132.838	-19.354
1600	4.989	53.482	49.438	6.471	182.860	129.495	-17.687
1700	5.004	53.785	49.685	6.970	18[illegible].578	126.168	-16.291
1800	5.025	54.071	49.921	7.472	182.284	122.858	-14.916
1900	5.056	54.344	50.146	7.976	181.977	119.567	-13.753
2000	5.097	54.604	50.363	8.483	181.658	116.288	-12.707
2100	5.150	54.854	50.571	8.995	181.327	113.029	-11.762
2200	5.218	55.095	50.771	9.514	180.988	109.785	-10.906
2300	5.301	55.329	50.964	10.040	180.639	106.556	-10.125
2400	5.401	55.557	51.151	10.574	180.281	103.343	-9.410
2500	5.518	55.779	51.331	11.120	179.918	100.145	-8.754
2600	5.655	55.998	51.507	11.679	179.550	96.960	-8.150
2700	5.810	56.215	51.677	12.252	179.178	93.791	-7.591
2800	5.984	56.429	51.843	12.841	178.804	90.635	-7.074
2900	6.178	56.642	52.005	13.449	178.430	87.492	-6.593
3000	6.390	56.855	52.163	14.078	178.059	84.363	-6.146
3100	6.620	57.069	52.318	14.728	177.688	81.247	-5.728
3200	6.866	57.283	52.469	15.402	177.322	78.144	-5.337
3300	7.127	57.498	52.619	16.101	176.962	75.048	-4.970
3400	7.402	57.715	52.765	16.828	176.608	71.966	-4.626
3453	7.552	57.830	52.842	17.224	176.423	70.337	-4.452
3453	7.552	57.830	52.842	17.224	169.481	70.337	-4.452
3500	7.688	57.933	52.910	17.582	168.3[illegible]2	68.998	-4.308
3600	7.984	58.154	53.052	18.366	168.066	66.167	-4.017
3700	8.288	58.377	53.193	19.179	167.719	63.344	-3.741
3800	8.596	58.602	53.333	20.023	167.463	60.525	-3.481
3900	8.908	58.829	53.471	20.899	167.239	57.711	-3.234
4000	9.220	59.059	53.608	21.805	167.045	54.906	-3.000
4100	9.531	59.290	53.743	22.743	166.883	52.108	-2.777
4200	9.838	59.524	53.878	23.711	166.751	49.311	-2.566
4300	10.138	59.759	54.012	24.710	166.650	46.514	-2.364
4400	10.431	59.995	54.145	25.739	166.579	43.721	-2.171
4500	10.714	60.233	54.278	26.796	166.556	40.929	-1.988
4600	10.986	60.471	54.410	27.881	166.521	38.138	-1.812
4700	11.244	60.710	54.542	28.993	166.533	35.346	-1.644
4800	11.489	60.950	54.673	30.129	166.569	32.552	-1.482
4900	11.719	61.189	54.803	31.290	166.630	29.766	-1.328
5000	11.932	61.428	54.933	32.473	166.713	26.970	-1.179
5100	12.130	61.666	55.063	33.676	166.816	24.174	-1.036
5200	12.311	61.903	55.192	34.898	166.938	21.378	-0.898
5300	12.475	62.139	55.321	36.138	167.078	18.574	-0.766
5400	12.623	62.374	55.450	37.393	167.233	15.767	-0.638
5500	12.754	62.607	55.578	38.662	167.402	12.962	-0.515
5600	12.869	62.838	55.705	39.943	167.583	10.157	-0.396
5700	12.968	63.066	55.832	41.235	167.775	7.342	-0.281
5800	13.052	63.293	55.959	42.536	167.976	4.526	-0.171
5900	13.122	63.516	56.085	43.845	168.185	1.709	-0.063
5960.67	13.157	63.650	56.161	44.641	168.315	0.000	0.000
5960.67	13.157	63.650	56.161	44.641			
6000	13.178	63.738	56.211	45.160			

ΔH°_{f0} = 185.196 kcal gfw^{-1}

$\Delta H^\circ_{f298.15}$ = 185.370 kcal gfw^{-1}

Ground State Configuration = $^6S_{2\frac{1}{2}}$

$S^\circ_{298.15}$ = 45.133 cal deg K^{-1}gfw^{-1}

$H^\circ_{298.15}-H^\circ_0$ = 1.481 kcal gfw^{-1}

Electronic Levels and Multiplicities

Spectroscopic energy levels from Moore.[1]

Heat of Formation

Third-Law calculation. Sherwood et al[2] vapor-pressure data.

Heat Capacity and Entropy

Calculated on monatomic-gas computer program.

References

1. Moore, C., Nat. Bur. Stds. (U.S.) Circ. 467, Vol. 3 (1958).
2. Sherwood, E. M. et al, J. Electrochem. Soc. 102, 650 (1955).

RHENIUM, MONATOMIC (Re) (IDEAL GAS) GFW = 186.22

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (kcal gfw)	ΔH_f (kcal gfw)	ΔF_f (kcal gfw)	log K_p
298.15	±0.000	±0.002	±0.002	±0.000	±1.500	±1.520	±1.110
1000	±0.000	±0.002	±0.003	±0.000	±1.520	±1.570	±0.340
2000	±0.000	±0.002	±0.003	±0.000	±1.820	±1.760	±0.192
3000	±0.001	±0.003	±0.003	±0.001	±2.570	±2.220	±0.160
3453	±0.002	±0.003	±0.003	±0.001	±3.140	±2.540	±0.160
3453	±0.002	±0.003	±0.003	±0.001	±4.640	±2.540	±0.160
4000	±0.003	±0.003	±0.003	±0.002	±5.270	±3.260	±0.180
5000	±0.006	±0.004	±0.003	±0.006	±8.130	±4.950	±0.220
5960.67	±0.009	±0.005	±0.003	±0.012	±12.940	±7.280	±0.270
5960.67	±0.009	±0.005	±0.003	±0.012			

TABLE 225

RHODIUM

REFERENCE STATE

Rh

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Rh from 0° to 2239°K, Liquid Rh from 2239° to 3996°K, Gaseous Rh from 3996° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.174			
298.15	5.940	7.530	7.530	0.000			
300	5.947	7.567	7.530	0.011			
400	6.262	9.323	7.767	0.622			
500	6.517	10.748	8.225	1.261			
600	6.747	11.957	8.749	1.925			
700	6.966	13.014	9.284	2.611			
800	7.180	13.958	9.811	3.318			
900	7.389	14.816	10.320	4.046			
1000	7.597	15.605	10.809	4.796			
1100	7.803	16.339	11.279	5.566			
1200	8.008	17.026	11.730	6.356			
1300	8.212	17.675	12.162	7.167			
1400	8.416	18.292	12.578	7.999			
1500	8.620	18.879	12.979	8.850			
1600	8.823	19.442	13.365	9.722			
1700	9.026	19.983	13.739	10.615			
1800	9.229	20.505	14.100	11.528			
1900	9.432	21.009	14.451	12.461			
2000	9.634	21.498	14.791	13.414			
2100	9.837	21.973	15.122	14.388			
2200	10.039	22.435	15.444	15.381			
2239	10.118	22.612	15.567	15.774			
2239	10.000	24.912	15.567	20.924			
2300	10.000	25.181	15.818	21.534			
2400	10.000	25.607	16.217	22.534			
2500	10.000	26.015	16.601	23.534			
2600	10.000	26.407	16.971	24.534			
2700	10.000	26.785	17.327	25.534			
2800	10.000	27.148	17.672	26.534			
2900	10.000	27.499	18.005	27.534			
3000	10.000	27.838	18.327	28.534			
3100	10.000	28.166	18.639	29.534			
3200	10.000	28.484	18.942	30.534			
3300	10.000	28.791	19.235	31.534			
3400	10.000	29.090	19.521	32.534			
3500	10.000	29.380	19.798	33.534			
3600	10.000	29.661	20.069	34.534			
3700	10.000	29.935	20.332	35.534			
3800	10.000	30.202	20.588	36.534			
3900	10.000	30.462	20.838	37.534			
3995.85	10.000	30.706	21.072	38.497			
3995.85	6.763	60.269	21.072	156.642			
4000	6.764	60.276	21.108	156.667			
4100	6.778	60.442	22.065	157.344			
4200	6.793	60.606	22.982	158.022			
4300	6.808	60.766	23.859	158.702			
4400	6.823	60.923	24.699	159.384			
4500	6.839	61.076	25.506	160.067			
4600	6.854	61.227	26.281	160.752			
4700	6.870	61.374	27.025	161.438			
4800	6.887	61.519	27.743	162.126			
4900	6.903	61.661	28.434	162.815			
5000	6.920	61.801	29.100	63.506			
5100	6.937	61.938	29.742	164.199			
5200	6.955	62.073	30.363	164.894			
5300	6.973	62.206	30.963	165.590			
5400	6.992	62.336	31.542	166.288			
5500	7.011	62.465	32.104	166.988			
5600	7.030	62.591	32.646	167.691			
5700	7.051	62.716	33.173	168.395			
5800	7.072	62.838	33.683	169.101			
5900	7.093	62.960	34.179	169.809			
6000	7.115	63.079	34.659	170.519			

15 December 1962

RCF

0^oK to 2239^oK	Crystal
2239^oK to 3996^oK	Liquid
3996^oK to 6000^oK	Ideal Monatomic Gas

$\Delta H^o_{f0} = 0$ $\Delta H^o_{f298.15} = 0$

$\Delta H^o_{s298.15} = 132.770$ kcal gfw^{-1} $S^o_{298.15} = 7.530$ cal deg K^{-1}gfw^{-1}

$T_m = 2239^oK$ $\Delta H_m = 5.150$ kcal gfw^{-1}

$T_b = 3996^oK$ $\Delta H_v = 118.145$ kcal gfw^{-1}

$H^o_{298.15} - H^o_0 = 1.174$ kcal gfw^{-1}

$C^o_p = 5.600 + 2.020 \times 10^{-3}T - 0.2334 \times 10^5 T^{-2}$ cal deg K^{-1}gfw^{-1}

$298.15^oK \leq T \leq 2239^oK$

$C^o_p = 10.000$ cal deg K^{-1}gfw^{-1} $2239^oK \leq T \leq 3996^oK$

Structure

An f. c. c. (A1) type.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Kelley and King's[1] S_{298} value adopted. High-temperature heat-capacity equation joined to low-temperature data. See volume 1, this study (section IVA22) for details.

Melting and Vaporization

Heat of fusion estimated. Melting-point values of several authors reported. Heat of vaporization calculated. Several vapor-pressure measurements reported. See volume 1, this study (section IVA22) for details

Reference

1. Kelley, K. K. and E. G. King, U. S. Bur. Mines, Bull. 592 (1961).

RHODIUM (Rh) (REFERENCE STATE) GFW = 102.91

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T (cal/°K gfw)	$-(F^o_T - H^o_{298})/T$ (cal/°K gfw)	$H^o_T - H^o_{298}$ (Kcal/gfw)	ΔH^o_f (Kcal/gfw)	ΔF^o_f (Kcal/gfw)	Log K_p
298.15	± 0.070	± 0.050	± 0.050	± 0.000			
1000	± 0.100	± 0.110	± 0.070	± 0.040			
2000	± 0.200	± 0.220	± 0.120	± 0.190			
2239	± 0.200	± 0.240	± 0.140	± 0.230			
2239	± 0.500	± 0.600	± 0.140	± 1.030			
3000	± 2.000	± 0.960	± 0.300	± 1.980			
3995.89	± 4.000	± 1.820	± 0.580	± 4.970			
3995.89	± 0.001	± 0.003	± 0.003	± 0.002			
5000	± 0.001	± 0.003	± 0.003	± 0.002			
6000	± 0.001	± 0.003	± 0.003	± 0.003			

TABLE 226

RHODIUM — IDEAL MONATOMIC GAS — **Rh**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Rh from 0° to 2239°K, Liquid Rh from 2239° to 3996°K, Gaseous Rh from 3996° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.483	132.461	132.461	INFINITE
298.15	5.023	44.388	44.388	0.000	132.770	121.781	-89.264
300	5.025	44.419	44.388	0.009	132.768	121.713	-88.664
400	5.174	45.883	44.587	0.518	132.666	118.042	-64.492
500	5.386	47.060	44.967	1.046	132.554	114.398	-50.001
600	5.618	48.062	45.402	1.596	132.441	110.778	-40.349
700	5.839	48.945	45.846	2.169	132.328	107.177	-33.461
800	6.034	49.738	46.284	2.763	132.215	103.591	-28.298
900	6.198	50.458	46.708	3.375	132.099	100.021	-24.287
1000	6.329	51.118	47.117	4.002	131.977	96.463	-21.081
1100	6.430	51.727	47.508	4.640	131.844	92.918	-18.460
1200	6.505	52.290	47.884	5.287	131.701	89.384	-16.278
1300	6.558	52.812	48.243	5.940	131.543	85.865	-14.435
1400	6.594	53.300	48.587	6.598	131.369	82.359	-12.856
1500	6.617	53.756	48.917	7.259	131.179	78.863	-11.490
1600	6.629	54.183	49.232	7.921	130.968	75.383	-10.296
1700	6.635	54.585	49.536	8.584	130.739	71.913	-9.245
1800	6.636	54.965	49.827	9.248	130.490	68.461	-8.312
1900	6.634	55.323	50.107	9.911	130.220	65.024	-7.479
2000	6.631	55.663	50.376	10.575	129.931	61.600	-6.731
2100	[illegible]	55.987	50.636	11.237	129.619	58.191	-6.056
2200	6.623	56.295	50.886	11.900	129.289	54.798	-5.443
2239	6.622	56.410	50.980	12.158	129.154	53.480	-5.220
2239	6.622	56.410	50.980	12.158	124.004	53.480	-5.220
2300	6.620	56.589	51.128	12.562	123.798	51.557	-4.899
2400	6.618	56.871	51.361	13.224	123.460	48.424	-4.409
2500	6.618	57.141	51.587	13.886	123.122	45.305	-3.960
2600	6.620	57.401	51.806	14.548	122.784	42.199	-3.547
2700	6.623	57.651	52.017	15.210	122.446	39.107	-3.165
2800	6.627	57.892	52.223	15.872	122.108	36.027	-2.812
2900	6.634	58.124	52.422	16.535	121.771	32.961	-2.484
3000	6.641	58.349	52.616	17.199	121.435	29.903	-2.178
3100	6.650	58.567	52.805	17.864	121.100	26.855	-1.893
3200	6.660	58.779	52.988	18.529	120.765	23.820	-1.627
3300	6.671	58.984	53.167	19.196	120.432	20.794	-1.377
3400	6.683	59.183	53.341	19.863	120.099	17.782	-1.143
3500	6.695	59.377	53.511	20.532	119.768	[illegible].774	-0.922
3600	6.708	59.566	53.676	21.202	119.438	11.781	-0.715
3700	6.721	59.750	53.838	21.874	119.110	8.794	-0.519
3800	6.735	59.929	53.996	22.547	118.783	5.820	-0.335
3900	6.749	60.104	54.150	23.221	118.457	2.849	-0.160
3995.89	6.763	60.269	54.295	23.872	118.145	0.000	0.000
3995.89	6.763	60.269	54.295	23.872			
4000	6.764	60.275	54.301	23.897			
4100	6.778	60.442	54.449	24.574			
4200	6.793	60.606	54.594	25.252			
4300	6.808	60.766	54.735	25.932			
4400	6.823	60.923	54.874	26.614			
4500	6.839	61.076	55.010	27.297			
4600	6.854	61.227	55.144	27.982			
4700	6.870	61.374	55.275	28.668			
4800	6.887	61.519	55.403	29.3			
4900	6.903	61.661	55.530	30.04			
5000	6.920	61.801	55.654	30.736			
5100	6.937	61.938	55.775	31.429			
5200	6.955	62.073	55.895	32.124			
5300	6.973	62.206	56.013	32.820			
5400	6.992	62.336	56.129	33.518			
5500	7.011	62.465	56.243	34.218			
5600	7.030	62.591	56.355	34.921			
5700	7.051	62.716	56.466	35.625			
5800	7.072	62.838	56.575	36.331			
5900	7.093	62.960	56.682	37.039			
6000	7.115	63.079	56.787	37.749			

15 December 1962 RGF

RHODIUM (Rh) (IDEAL MONATOMIC GAS) gfw = 102.91

ΔH^o_{f0} = 132.461 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 132.770 kcal gfw^{-1}

Ground State Configuration = $^4F_{4\frac{1}{2}}$

$S^o_{298.15}$ = 44.388 cal deg K^{-1}gfw^{-1}

$H^o_{298.15}-H^o_0$ = 1.483 kcal gfw^{-1}

Electronic Levels and Multiplicities

Spectroscopic energy levels from Moore.[1]

Heat of Formation

An average of two determinations adopted. See volume 1, this study (section IVA22) for details.

Heat Capacity and Entropy

Calculated on monatomic-gas computer program.

Reference

1. Moore, C., Nat. Bur. Stds. (U.S.) Circ. 467, Vol. 3 (May 1958).

RHODIUM, MONATOMIC (Rh) (IDEAL GAS) GFW = 102.91

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw			Kcal/gfw			
	C^o_p	S^o_T	$-(F^o_T - H^o_{298})/T$	$H^o_T - H^o_{298}$	ΔH^o_f	ΔF^o_f	Log K_p
298.15	± 0.000	± 0.002	± 0.002	±0.000	±1.600	± 1.620	± 1.190
1000	± 0.001	± 0.002	± 0.003	±0.000	±1.640	± 1.670	± 0.360
2000	± 0.001	± 0.003	± 0.003	±0.001	±1.790	± 1.850	± 0.200
2239	± 0.001	± 0.003	± 0.003	±0.001	±1.830	± 1.920	± 0.190
2239	± 0.001	± 0.003	± 0.003	±0.001	±2.630	± 1.920	± 0.190
3000	± 0.001	± 0.003	± 0.003	±0.001	±3.580	± 2.520	± 0.180
3995.89	± 0.001	± 0.003	± 0.003	±0.001	±6.570	± 3.930	± 0.210
3995.89	± 0.001	± 0.003	± 0.003	±0.002			
4000	± 0.001	± 0.003	± 0.003	±0.002			
5000	± 0.001	± 0.003	± 0.003	±0.002			
6000	± 0.001	± 0.003	± 0.003	±0.003			

TABLE 227

SCANDIUM | **REFERENCE STATE** | **Sc**

**Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Sc from 0° to 1812°K
Liquid Sc from 1812° to 3021°K, Gaseous Sc from 3021° to 6000°K**

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.280			
298.15	6.000	9.000	9.000	0.000			
300	6.002	9.037	9.000	0.011			
400	6.110	10.778	9.236	0.617			
500	6.218	12.154	9.688	1.233			
600	6.326	13.297	10.197	1.860			
700	6.434	14.280	10.711	2.498			
800	6.542	15.146	11.212	3.147			
900	6.650	15.923	11.693	3.807			
1000	6.758	16.629	12.152	4.477			
1100	6.866	17.278	12.589	5.158			
1200	6.974	17.880	13.005	5.850			
1300	7.082	18.443	13.402	6.553			
1400	7.190	18.972	13.782	7.267			
1500	7.328	19.471	14.144	7.991			
1600	7.406	19.946	14.492	8.726			
1608	7.415	19.984	14.520	8.786			
1608	8.000	20.202	14.520	9.136			
1700	8.000	20.647	14.840	9.872			
1800	8.000	21.104	15.175	10.672			
1812	8.000	21.158	15.215	10.768			
1812	8.000	23.238	15.215	14.536			
1900	8.000	23.618	15.596	15.242			
2000	8.000	24.028	16.007	16.042			
2100	8.000	24.418	16.398	16.842			
2200	8.000	24.790	16.771	17.642			
2300	8.000	25.146	17.128	18.442			
2400	8.000	25.486	17.468	19.242			
2500	8.000	25.813	17.796	20.042			
2600	8.000	26.127	18.111	20.842			
2700	8.000	26.429	18.413	21.642			
2800	8.000	26.720	18.705	22.442			
2900	8.000	27.000	18.986	23.242			
3000	8.000	27.271	19.257	24.042			
3021	8.000	27.326	19.312	24.210			
3021	6.248	53.651	19.312	103.731			
3100	6.397	53.815	20.193	104.229			
3200	6.599	54.021	21.246	104.879			
3300	6.810	54.227	22.242	105.549			
3400	7.031	54.434	23.187	106.241			
3500	7.259	43.641	24.082	106.955			
3600	7.492	54.849	24.934	107.693			
3700	7.730	55.057	25.745	108.454			
3800	7.969	55.267	26.520	109.239			
3900	8.208	55.477	27.260	110.048			
4000	8.446	55.688	27.968	110.881			
4100	8.680	55.899	28.646	111.737			
4200	8.909	56.111	29.298	112.616			
4300	9.132	56.323	29.923	113.518			
4400	9.347	56.536	30.526	114.442			
4500	9.554	56.748	31.106	115.388			
4600	9.750	56.960	31.666	116.353			
4700	9.936	57.172	32.207	117.337			
4800	10.111	57.383	32.729	11[illegible]340			
4900	10.274	57.593	33.234	119.359			
5000	10.425	57.802	33.723	120.394			
5100	10.563	58.010	34.197	121.444			
5200	10.689	58.216	34.657	122.506			
5300	10.803	58.421	35.104	123.581			
5400	10.905	58.624	35.538	124.667			
5500	10.994	58.825	35.959	125.762			
5600	11.072	59.024	36.370	126.865			
5700	11.139	59.220	36.768	127.976			
5800	11.19[illegible]	59.415	37.158	129.093			
5900	11.242	59.606	37.536	130.215			
6000	11.279	59.796	37.906	131.341			

May 1962 | RCF

SCANDIUM (Sc) (REFERENCE STATE) gfw = 44.96

0 °K to 1812 °K Crystal

1812 °K to 3021 °K Liquid

3021 °K to 6000 °K Ideal Monatomic Gas

$\Delta H^\circ_{f0} = 0$

$\Delta H^\circ_{f298.15} = 0$

$\Delta H^\circ_{s298.15} = 89.500$ Kcal gfw^{-1}

$S^\circ_{298.15} = 9.0$ cal deg^{-1} gfw^{-1}

$T_t = 1608$ °K

$\Delta H_t = 0.350$ Kcal gfw^{-1}

$T_m = 1812$ °K

$\Delta H_m = 3.770$ Kcal gfw^{-1}

$T_b = 3021$ °K

$\Delta H_v = 79.521$ Kcal gfw^{-1}

$H^\circ_{298.15} - H^\circ_0 = 1.280$ Kcal gfw^{-1}

$C^\circ_{P0} = 5.68 + 1.08 \times 10^{-3}\,T$ cal deg K^{-1} gfw^{-1} $\quad 298.15\text{°K} \le 1608\text{ °K}$

$C^\circ_p = 8.0$ cal deg K^{-1} gfw^{-1} $\quad 1608\text{ °K} \le 3021\text{ °K}$

Structure

Low temperature form is h. c. p.; high temperature form is probably b. c. c.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Low temperature data estimated by Kelley and King[1]. High temperature data estimated by Kelley[2].

Melting

Melting point by Spedding et al.[3]

Vaporization

Based on data of Spedding et al.[3]

Further details given by Barriault et al.[4]

References

1. Kelley, K., E. King, Bur. Mines. Bull. 592 (1961).
2. Kelley, K., Bur. Mines. Bull. 584 (1960).
3. Spedding, F. H., et al, Trans AIME 218 608 (1960).
4. Barriault, R., et al, ASD-TR-61-260(May 1962), Pt. I.

SCANDIUM (Sc) (REFERENCE STATE) GFW = 44.96

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0				± .040			
298.15	± 0.200	± 0.500	± 0.500	± 0.000			
1000	± 0.350	± 0.830	± 0.640	± 0.190			
1608	± 0.500	± 1.090	± 0.800	± 0.460			
1608	± 1.000	± 1.150	± 0.800	± 0.560			
1812	± 1.500	± 1.300	± 0.850	± 0.810			
1812	± 0.400	± 1.410	± 0.850	± 1.010			
3021	± 2.300	± 2.100	± 1.220	± 2.640			
3021	± 0.001	± 0.002					
4000	± 0.002	± 0.003					
5000	± 0.002	± 0.003					
6000	± 0.002	± 0.003					

TABLE 228

SCANDIUM — **IDEAL MONATOMIC GAS** — **Sc**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Sc from 0° to 1812°K, Liquid Sc from 1812° to 3021°K, Gaseous Sc from 3021° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.674	89.106	89.106	INFINITE
298.15	5.283	41.750	41.750	0.000	89.500	79.736	-58.445
300	5.279	41.783	41.750	0.010	89.499	79.665	-58.033
400	5.148	43.281	41.955	0.530	89.413	76.412	-41.748
500	5.085	44.422	42.339	1.042	89.309	73.174	-31.983
600	5.049	45.346	42.765	1.548	89.188	69.959	-25.480
700	5.028	46.122	43.191	2.052	89.054	66.763	-20.843
800	5.014	46.793	43.600	2.554	88.907	63.590	-17.371
900	5.004	47.383	43.988	3.055	88.748	60.434	-14.675
1000	4.997	47.909	44.355	3.555	88.578	57.297	-12.522
1100	4.992	48.386	44.700	4.054	88.396	54.178	-10.764
1200	4.989	48.820	45.025	4.553	88.203	51.076	-9.302
1300	4.988	49.219	45.333	5.052	87.999	47.990	-8.067
1400	4.989	49.589	45.624	5.551	87.784	44.921	-7.012
1500	4.993	49.933	45.900	6.050	87.559	41.866	-6.100
1600	5.001	50.256	46.162	6.550	87.324	38.828	-5.303
1608	5.002	50.280	46.182	6.590	87.304	38.587	-5.244
1608	5.0[illegible]	50.280	46.182	6.590	86.954	38.587	-5.244
1700	5.014	50.559	46.412	7.050	86.678	35.828	-4.606
1800	5.0[illegible]	50.846	46.650	7.553	86.381	32.845	-3.988
1812	5.0[illegible]7	50.879	46.677	7.614	86.346	32.490	-3.919
1812	[illegible]	50.879	46.677	7.614	82.576	32.490	-3.919
1900	5.062	51.119	46.878	8.058	82.316	30.064	-3.458
2000	5.099	51.380	47.097	8.566	82.024	27.320	-2.985
2100	5.148	51.630	47.307	9.078	81.736	24.591	-2.559
2200	5.208	51.870	47.509	9.595	81.453	21.876	-2.173
2300	5.282	52.103	47.704	10.120	81.178	19.175	-1.822
2400	5.369	52.330	47.892	10.652	80.910	16.482	-1.501
2500	5.472	52.551	48.074	11.19[illegible]	80.652	13.805	-1.207
2600	5.589	52.768	48.250	11.747	80.405	11.139	-0.936
2700	5.722	52.981	48.421	12.312	80.170	8.478	-0.686
2800	5.869	53.192	48.588	12.892	79.950	5.828	-0.455
2900	6.032	53.401	48.750	13.487	79.745	3.184	-0.240
3000	6.208	53.608	48.909	14.099	79.557	0.544	-0.040
3021	6.248	53.651	48.941	14.231	79.521	0.000	0.000
3021	6.248	53.651	48.941	14.231			
3100	6.397	53.815	49.064	14.729			
3200	6.599	54.021	49.215	15.379			
3300	6.810	54.227	49.364	16.049			
3400	7.031	54.434	49.510	16.741			
3500	7.259	54.641	49.654	17.455			
3600	7.492	54.849	49.795	18.193			
3700	7.730	55.057	49.935	18.954			
3800	7.969	55.267	50.072	19.739			
3900	8.208	55.477	50.208	20.548			
4000	8.446	55.688	50.342	21.381			
4100	8.680	55.899	50.475	22.237			
4200	8.909	56.111	50.607	23.116			
4300	9.132	56.323	50.738	24.018			
4400	9.347	56.536	50.867	24.942			
4500	9.554	56.748	50.995	25.888			
4600	9.750	56.960	51.123	26.8[illegible]			
4700	9.936	57.172	51.249	27.8[illegible]			
4800	10.111	57.383	51.375	28.840			
4900	10.274	57.593	51.499	29.859			
5000	10.425	57.802	51.623	30.894			
5100	10.563	58.010	51.747	31.944			
5200	10.689	58.216	51.869	33.006			
5300	10.803	58.421	51.991	34.081			
5400	10.905	58.624	52.112	35.167			
5500	10.994	58.825	52.232	36.262			
5600	11.072	59.024	52.351	37.365			
5700	11.139	59.220	52.470	38.476			
5800	11.196	59.415	52.588	39.593			
5900	11.242	59.606	52.706	40.715			
6000	11.279	59.796	52.822	41.841			

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SCANDIUM, MONATOMIC (Sc) (IDEAL GAS) gfw = 44.96

ΔH^o_{f0} = 89.106 Kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 89.500 Kcal gfw^{-1}

Ground State Configuration $^2D_{1-1/2}$

$S^o_{298.15}$ = 41.750 cal degK^{-1} gfw^{-1}

$H^o_{298.15} - H^o_0$ = 1.674 Kcal gfw^{-1}

Electronic levels and multiplicities

Source of Data

Energy Leve... ...ore[1].

Heat of Formation

Based on vaporization data of Spedding *et al*[2].

Heat Capacity and Entropy

Calculated using monatomic gas computer program.

Further details given by Barriault *et al*[3].

References

1. Moore, C., Atomic Energy Levels, Vol. 1, Nat. Bur. Stds. (1949).
2. Spedding, F. H., *et al*, Trans. AIME 218, 608 (1960).
3. Barriault, R. *et al*, ASD TR-61-260 (May 1962), Pt. I.

SCANDIUM, MONATOMIC (Sc) (IDEAL GAS) GFW = 44.96

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T (cal/°K gfw)	$-(F^o_T - H^o_{298})/T$ (cal/°K gfw)	$H^o_T - H^o_{298}$ (Kcal/gfw)	ΔH_f (Kcal/gfw)	ΔF_f (Kcal/gfw)	Log K_p
298.15	± 0.000	± 0.002	± 0.002	± 0.000	± 0.500	± 0.650	± 0.480
1000	± 0.000	± 0.002	± 0.002	± 0.000	± 0.500	± 1.060	± 0.230
1608	± 0.000	± 0.002	± 0.002	± 0.000	± 0.500	± 1.790	± 0.240
1608	± 0.000	± 0.002	± 0.002	± 0.000	± 0.600	± 1.790	± 0.240
1812	± 0.000	± 0.002	± 0.003	± 0.000	± 0.850	± 1.940	± 0.230
1812	± 0.000	± 0.002	± 0.003	± 0.000	± 1.050	± 1.940	± 0.230
3021	± 0.001	± 0.002	± 0.003	± 0.001	± 2.680	± 3.690	± 0.270
3021	± 0.001	± 0.002	± 0.003	± 0.001			
4000	± 0.002	± 0.003	± 0.003	± 0.002			
5000	± 0.002	± 0.003	± 0.003	± 0.004			
6000	± 0.002	± 0.003	± 0.003	± 0.005			

TABLE 229

SILICON — **REFERENCE STATE** — **Si**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Si from 0° to 1690°K, Liquid Si from 1690° to 3566°K, Gaseous Si from 3566° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-0.769			
298.15	4.739	4.530	4.530	0.000			
300	4.754	4.559	4.530	0.009			
400	5.330	6.017	4.725	0.517			
500	5.634	7.242	5.109	1.066			
600	5.831	8.287	5.554	1.640			
700	5.981	9.198	6.011	2.231			
800	6.114	10.005	6.460	2.836			
900	6.232	10.732	6.895	3.453			
1000	6.340	11.394	7.313	4.082			
1100	6.441	12.003	7.712	4.721			
1200	6.536	12.568	8.093	5.370			
1300	6.628	13.095	8.458	6.028			
1400	6.718	13.589	8.807	6.695			
1500	6.806	14.056	9.142	7.372			
1600	6.8[illegible]	14.498	9.463	8.057			
1690	6.97[illegible]	14.877	9.741	8.681			
1690	6.973	21.948	9.741	20.631			
1700	6.981	21.989	9.813	20.700			
1800	7.068	22.391	10.501	21.403			
1900	7.15[illegible]	22.775	11.137	22.114			
2000	[illegible]	23.143	11.728	22.831			
2100	7.1[illegible]5	23.492	12.280	23.546			
2200	7.155	23.825	12.797	24.262			
2300	7.155	24.143	13.283	24.977			
2400	7.1[illegible]5	24.448	13.742	25.693			
2500	7.155	24.740	14.176	26.408			
2600	7.155	25.020	14.588	27.124			
2700	7.155	25.290	14.979	27.839			
2800	7.155	25.550	15.352	28.555			
2900	7.155	25.802	15.708	29.270			
3000	7.155	26.044	16.049	29.986			
3100	7.[illegible]55	26.279	16.375	30.701			
3200	7.155	26.506	16.688	31.417			
3300	7.155	26.726	16.989	32.132			
3400	7.155	26.940	17.279	32.848			
3500	7.155	27.147	17.558	33.563			
3565.77	7.155	27.280	17.736	34.033			
3565.77	5.506	52.939	17.736	125.528			
3600	5.508	52.992	18.071	125.716			
3700	5.513	53.143	19.017	126.267			
3800	5.516	53.291	19.917	126.819			
3900	5.519	53.434	20.774	127.371			
4000	5.521	53.574	21.593	127.922			
4100	5.522	53.710	22.374	128.475			
4200	5.522	53.843	23.123	129.027			
4300	5.522	53.973	23.838	129.579			
4400	5.522	54.100	24.525	130.131			
4500	5.521	54.224	25.184	130.683			
4600	5.520	54.345	25.816	131.236			
4700	5.518	54.464	26.424	131.787			
4800	5.517	54.580	27.009	132.[illegible]9			
4900	5.515	54.694	27.573	132.8[illegible]1			
5000	5.513	54.805	28.117	133.442			
5100	5.512	54.915	28.642	133.994			
5200	5.510	55.022	29.148	134.545			
5300	5.509	55.126	29.637	135.096			
5400	5.508	55.229	30.110	135.646			
5500	5.508	55.331	30.568	136.197			
5600	5.507	55.430	31.011	136.748			
5700	5.508	55.527	31.439	137.299			
5800	5.509	55.623	31.856	137.850			
5900	5.511	55.717	32.260	138.401			
6000	5.514	55.810	32.651	138.952			

15 March 1963 HLS

$0^{o}K$ to $1690^{o}K$	Crystal
$1690^{o}K$ to $3565.77^{o}K$	Liquid
$3565.77^{o}K$ to $6000^{o}K$	Ideal Monatomic Gas

$\Delta H_{f0}^{o} = 0$

$\Delta H_{f298.15}^{o} = 0$

$\Delta H_{s298.15} = 108.407$ Kcal gfw^{-1}

$S_{298.15}^{o} = 4.53$ cal $degK^{-1}$ gfw^{-1}

$T_m = 1690^{o}K$

$\Delta H_m = 11.950$ Kcal gfw^{-1}

$T_b = 3565.77^{o}K$

$\Delta H_v = 91.495$ Kcal gfw^{-1}

$H_{298.15}^{o} - H_0^{o} = 0.769$ Kcal gfw^{-1}

C_p^{o} data was selected and smoothed (See below).

Structure

Silicon has a cubic A4 (i. e., diamond type) structure.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Low temperature data from Stull and Sinke.[1] Kelley's[2] equation used to 600°K. From 600° to 1900°K, the data of Kantor et al[3] joined Kelley's data. Above 1900°K estimated data were used.

Melting

Data of Kantor et al[3] were used.

Heat of Sublimation

Several sources were reviewed. See gas table (table 230), this volume, also see volume 1, this study (section IVA25).

References

1. Stull, D. R. and G. C. Sinke, Thermodynamic Properties of the Elements (1956).
2. Kelley, K. K., Bur. Mines, Bull. 584 (1960).
3. Kantor, P. B., O. M. Kisil and E. M. Fomichov, Ukr. Fiz. Zh. 5, 358-362 (1960).

SILICON (Si) (REFERENCE STATE) GFW = 28.09

SUMMARY OF UNCERTAINTY ESTIMATES

	cal/°K gfw			Kcal/gfw			
T, °K	C_p^{o}	S_T^{o}	$-(F_T^{o} - H_{298}^{o})/T$	$H_T^{o} - H_{298}^{o}$	ΔH_f^{o}	ΔF_f^{o}	Log K_p
298.15	± 0.100	± 0.050	± 0.050	± 0.000			
1000	± 0.100	± 0.171	± 0.101	± 0.070			
1000	± 0.500	± 0.171	± 0.101	± 0.070			
1690	± 0.500	± 0.433	± 0.188	± 0.415			
1690	± 0.500	± 0.552	± 0.188	± 0.615			
1900	± 0.500	± 0.610	± 0.231	± 0.720			
1900	± 1.000	± 0.610	± 0.231	± 0.720			
2000	± 1.000	± 0.662	± 0.251	± 0.820			
3000	± 1.000	± 1.067	± 0.460	± 1.820			
3565.77	± 1.000	± 1.240	± 0.571	± 2.386			

SILICON **IDEAL MONATOMIC GAS** **Si**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Si from 0° to 1690°K, Liquid Si from 1690° to 3566°K, Gaseous Si from 3566° to 6000°K

	cal/°K gfw			Kcal/gfw			
T, °K	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.805	107.371	107.371	INFINITE
298.15	5.319	40.123	40.123	0.000	108.407	97.795	-71.682
300	5.315	40.156	40.123	0.010	108.408	97.729	-71.192
400	5.166	41.662	40.330	0.533	108.423	94.165	-51.447
500	5.095	42.806	40.715	1.046	108.387	90.604	-39.601
600	5.056	43.731	41.143	1.553	108.320	87.054	-31.708
700	5.033	44.509	41.570	2.057	108.233	83.516	-26.074
800	5.019	45.180	41.980	2.560	108.131	79.991	-21.851
900	5.012	45.770	42.369	3.061	108.015	76.480	-18.571
1000	5.012	46.299	42.736	3.563	107.888	72.984	-15.950
1100	5.017	46.776	43.082	4.064	107.750	69.500	-13.808
1200	5.027	47.213	43.408	4.566	107.603	66.029	-12.025
1300	5.043	47.616	43.717	5.070	107.449	62.570	-10.519
1400	5.063	47.991	44.009	5.575	107.287	59.124	-9.229
1500	5.087	48.341	44.286	6.082	107.117	55.691	-8.114
1600	5.113	48.670	44.550	6.592	106.942	52.268	-7.139
1690	5.139	48.950	44.777	7.054	106.780	49.196	-6.362
1690	5.139	48.950	44.777	7.054	94.830	49.196	-6.362
1700	5.142	48.981	44.801	7.105	94.812	48.927	-6.290
1800	5.172	49.276	45.042	7.621	94.625	46.233	-5.613
1900	5.202	49.556	45.272	8.139	94.432	43.551	-5.009
2000	5.232	49.824	45.493	8.661	94.237	40.877	-4.467
2100	[illegible].261	50.080	45.705	9.186	94.047	38.215	-3.977
2200	5.289	50.325	45.910	9.713	93.858	35.558	-3.532
2300	5.316	50.561	46.107	10.243	93.673	32.912	-3.127
2400	5.[illegible]41	50.787	46.297	10.776	93.490	30.275	-2.757
2500	5.[illegible]65	51.006	46.481	11.312	93.311	27.645	-2.417
2600	5.386	51.217	46.659	11.849	93.132	25.022	-2.103
2700	5.406	51.420	46.832	12.389	92.957	22.404	-1.813
2800	5.424	51.617	46.999	12.930	92.782	19.795	-1.545
2900	5.440	51.808	47.162	13.473	92.610	17.190	-1.295
3000	5.454	51.993	47.320	14.018	92.439	14.594	-1.063
3100	5.467	52.172	47.473	14.564	92.270	12.003	-0.846
3200	5.478	52.345	47.623	15.111	92.101	9.415	-0.643
3300	5.487	52.514	47.769	15.660	91.935	6.833	-0.453
3400	5.495	52.678	47.911	16.209	91.768	4.258	-0.274
3500	5.502	52.837	48.049	16.759	91.603	1.689	-0.105
3565.77	5.506	52.939	48.138	17.121	91.495	0.000	0.000
3565.77	5.506	52.939	48.138	17.121			
3600	5.508	52.992	48.184	17.309			
3700	5.513	53.143	48.316	17.860			
3800	5.516	53.291	48.445	18.412			
3900	5.519	53.434	48.571	18.964			
4000	5.521	53.574	48.695	19.515			
4100	5.522	53.710	48.815	20.068			
4200	5.522	53.843	48.934	20.620			
4300	5.522	53.973	49.049	21.172			
4400	5.522	54.100	49.163	21.724			
4500	5.521	54.224	49.274	22.276			
4600	5.520	54.345	49.383	22.829			
4700	5.518	54.464	49.489	23.380			
4800	5.517	54.580	49.594	23.932			
4900	5.515	54.694	49.697	24.484			
5000	5.513	54.805	49.798	25.035			
5100	5.512	54.915	49.898	25.587			
5200	5.510	55.022	49.995	26.138			
5300	5.509	55.126	50.091	26.689			
5400	5.508	55.229	50.185	27.239			
5500	5.508	55.331	50.278	27.790			
5600	5.507	55.430	50.369	28.341			
5700	5.508	55.527	50.458	28.892			
5800	5.509	55.623	50.547	29.443			
5900	5.511	55.717	50.634	29.994			
6000	5.514	55.810	50.719	30.545			

15 March 1963 HLS

ΔH^o_{f0} = 107.371 Kcal gfw^{-1}

Ground State Configuration $^3P_0$

$H^o_{298.15}-H^o_0$ = 1.805 Kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 108.407 Kcal gfw^{-1}

$S^o_{298.15}$ = 40.123 cal degK^{-1} gfw^{-1}

Electronic Levels and Multiplicities

All energy levels from Moore[1] were used to calculate functions in an earlier report.[2]

Heat of Formation

Based on vapor pressure data of Davis et al.[3] Several other sources of data were reviewed and are discussed in volume 1, this study (section IVA25).

Heat Capacity and Entropy

Calculated in an earlier report.[2]

References

1. Moore, C., Nat. Bur. Std. (U.S.), Circ. 467, Vol. 1 (1949).
2. Barriault, R. J. et al, Thermodynamics of Certain Refractory Compounds Pt. I, Vol. 1, ASD TR-61-260 (May 1962).
3. Davis, S. G., D. F. Anthrop and A. W. Searcy, J. Chem. Phys. 34, 659 (1961).

SILICON, MONATOMIC (Si) (IDEAL GAS) GFW = 28.09

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T	$-(F^o_T - H^o_{298})/T$	$H^o_T - H^o_{298}$ (Kcal gfw)	ΔH_f	ΔF_f	Log K_p
298.15	± 0.000	± 0.002	± 0.002	± 0.000	± 3.000		
1000	± 0.000	± 0.002	± 0.002	± 0.000			
2000	± 0.000	± 0.002	± 0.002	± 0.000			
3000	± 0.000	± 0.002	± 0.003	± 0.001			
4000	± 0.000	± 0.002	± 0.003	± 0.001			
5000	± 0.000	± 0.002	± 0.003	± 0.001			
6000	± 0.001	± 0.003	± 0.003	± 0.002			

TABLE 231

STRONTIUM | **REFERENCE STATE** | **Sr**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Sr from 0° to 1045°K, Liquid Sr from 1045° to 1641°K, Gaseous Sr from 1641° to 6000°K

T, °K	cal/°K gfw C_p°	cal/°K gfw S_T°	cal/°K gfw $-(F_T^\circ - H_{298}^\circ)/T$	Kcal/gfw $H_T^\circ - H_{298}^\circ$	Kcal/gfw ΔH_f°	Kcal/gfw ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.550			
298.15	6.400	12.500	12.500	0.000			
300	6.407	12.540	12.501	0.012			
400	6.807	14.438	12.757	0.673			
500	7.207	15.999	13.253	1.373			
600	7.607	17.349	13.826	2.114			
700	8.007	18.551	14.416	2.895			
800	8.407	19.647	15.003	3.715			
862	8.655	20.283	15.359	4.244			
862	9.160	20.515	15.359	4.444			
900	9.160	20.910	15.586	4.792			
1000	9.160	21.875	16.167	5.708			
1045	9.160	22.278	16.421	6.120			
1045	7.800	24.163	16.421	8.090			
1100	7.800	24.563	16.818	8.519			
1200	7.800	25.242	17.493	9.299			
1300	7.800	25.866	18.113	10.079			
1400	7.800	26.444	18.688	10.859			
1500	7.800	26.982	19.223	11.639			
1600	7.800	27.486	19.724	12.419			
1641	7.800	27.680	19.922	12.731			
1641	4.977	47.797	19.922	45.743			
1700	[illegible].981	47.975	20.895	46.036			
1800	4.991	48.260	22.407	46.535			
1900	5.007	48.530	23.775	47.035			
2000	5.031	48.787	25.019	47.537			
2100	5.065	49.033	26.156	48.041			
2200	5.111	49.270	27.202	48.550			
2300	5.171	49.499	28.167	49.064			
2400	5.249	49.720	29.060	49.58[illegible]			
2500	5.345	49.936	29.890	50.114			
2600	5.461	50.148	30.666	50.654			
2700	5.600	50.357	31.391	51.207			
2800	5.762	50.563	32.072	51.775			
2900	5.949	50.769	32.713	52.361			
3000	6.159	50.974	33.319	52.966			
3100	6.394	51.180	33.892	53.593			
3200	6.653	51.387	34.435	54.245			
3300	6.933	51.596	34.952	54.924			
3400	7.235	51.807	35.444	55.633			
3500	7.556	52.021	35.915	56.372			
3600	7.894	52.239	36.365	57.144			
3700	8.247	52.460	36.797	57.951			
3800	8.611	52.685	37.213	58.794			
3900	8.984	52.913	37.612	59.674			
4000	9.364	53.145	37.997	60.591			
4100	9.747	53.381	38.370	61.547			
4200	10.131	53.621	38.730	62.541			
4300	10.513	53.864	39.080	63.57[illegible]			
4400	10.891	54.110	39.418	64.64[illegible]			
4500	11.262	54.359	39.748	65.751			
4600	11.625	54.610	40.068	66.895			
4700	11.979	54.864	40.380	68.076			
4800	12.320	55.170	40.684	69.[illegible]			
4900	12.650	55.377	40.981	70.539			
5000	12.965	55.636	41.272	71.820			
5100	13.267	55.896	41.556	73.132			
5200	13.554	56.156	41.833	74.473			
5300	13.826	56.417	42.107	75.842			
5400	14.082	56.678	42.374	77.238			
5500	14.324	56.938	42.636	78.658			
5600	14.550	57.198	42.894	80.102			
5700	14.762	57.458	43.148	81.568			
5800	14.959	57.716	43.396	83.054			
5900	51.141	57.974	43.642	84.559			
6000	15.309	58.230	43.883	86.081			

May 1962 RCF

STRONTIUM (Sr) (REFERENCE STATE) gfw = 87.63

0 °K to 1045 °K Crystal

1045 °K to 1641 °K Liquid

1641 °K to 6000 °K Ideal Monatomic Gas

$\Delta H^o_{f0} = 0$ $\Delta H^o_{f298.15} = 0$

$\Delta H^o_{s298.15} = 39.070$ Kcal gfw^{-1} $S^o_{298.15} = 12.5$ cal deg K^{-1} gfw^{-1}

$T_t = 862$ °K $\Delta H_t = 0.200$ Kcal gfw^{-1}

$T_m = 1045$ °K $\Delta H_m = 1.970$ Kcal gfw^{-1}

$T_b = 1641$ °K $\Delta H_v = 33.012$ Kcal gfw^{-1}

$H^o_{298.15} - H^o_0 = 1.550$ Kcal gfw^{-1}

$C^o_p = 5.207 + 4.00 \times 10^{-3} T$ cal deg K^{-1} gfw^{-1} $298.15°K \leq T \leq 862°K$

$C^o_p = 9.16$ cal deg K^{-1} gfw^{-1} $862°K \leq T \leq 1045°K$

$C^o_p = 7.80$ cal deg K^{-1} gfw^{-1} $1045°K \leq T \leq 1641°K$

Structure

Low-temperature form (α - Sr) has f.c.c. structure; high-temperature form (γ - Sr) has b.c.c. structure.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Low-temperature data estimated by Kelley and King.[1] High-temperature lata were estimated.

Melting

Average of three melting point values was used.

Vaporization-pressure determinations were averaged; see Barriault[2] for details.

References

1. Kelley, K. and E. King, Bur. Mines. Bull. 592 (1961).

2. Barriault, R., et al, ASD-TR-61-260 (May 1962), Pt. 1.

STRONTIUM (Sr) (REFERENCE STATE) GFW = 87.63

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T (cal/°K gfw)	$-(F^o_T - H^o_{298})/T$ (cal/°K gfw)	$H^o_T - H^o_{298}$ (Kcal/gfw)	ΔH^o_f (Kcal/gfw)	ΔF^o_f (Kcal/gfw)	Log K_p
298.15	± 0.200	± 0.500	± 0.500	± 0.000			
862	± 0.300	± 0.610	± 0.540	± 0.060			
862	± 0.600	± 0.730	± 0.540	± 0.160			
1045	± 1.000	± 0.760	± 0.580	± 0.190			
1045	± 0.500	± 0.910	± 0.580	± 0.340			
1641	± 1.500	± 1.130	± 0.740	± 0.640			
1641	± 0.000	± 0.002					
2000	± 0.000	± 0.002					
3000	± 0.001	± 0.002					
4000	± 0.002	± 0.003					
5000	± 0.003	± 0.003					
6000	± 0.003	± 0.003					

TABLE 232

STRONTIUM **IDEAL MONATOMIC GAS** **Sr**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Sr from 0° to 1045°K, Liquid Sr from 1045°K to 1641°K, Gaseous Sr from 1641° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.481	39.139	39.139	INFINITE
298.15	4.968	39.325	39.325	0.000	39.070	31.072	-22.775
300	4.968	39.356	39.325	0.009	39.067	31.023	-22.599
400	4.968	40.785	39.520	0.506	38.903	28.365	-15.497
500	4.968	41.894	39.888	1.003	38.700	25.752	-11.256
600	4.968	42.799	40.300	1.500	38.456	23.186	-8.445
700	4.968	43.565	40.713	1.996	38.171	20.662	-6.451
800	4.968	44.229	41.122	2.493	37.848	18.183	-4.967
862	4.968	44.600	41.350	2.801	37.627	16.666	-4.225
862	4.968	44.600	41.350	2.801	37.427	16.666	-4.225
900	4.968	44.814	41.492	2.990	37.268	15.755	-3.826
1000	4.968	45.337	41.850	3.487	36.849	13.387	-2.926
1045	4.968	45.556	42.005	3.711	36.661	12.335	-2.580
1045	4.968	45.556	42.005	3.711	34.691	12.335	-2.580
1100	4.968	45.811	42.189	3.984	34.535	11.162	-2.218
1200	4.968	46.243	42.509	4.481	34.252	9.051	-1.648
1300	4.969	46.641	42.812	4.977	33.968	6.961	-1.170
1400	4.969	47.009	43.099	5.474	33.685	4.895	-0.764
1500	4.971	47.352	43.371	5.971	33.402	2.848	-0.415
1600	4.975	47.673	43.630	6.496	33.120	0.82	-0.112
1641	4.977	47.797	43.731	6.673	3[illegible].[illegible]12	0.0[illegible]	0.000
1641	4.977	47.797	43.731	6.673			
1700	4.[illegible]81	47.975	43.877	6.966			
1800	4.991	48.260	44.112	7.465			
1900	5.007	48.530	44.338	7.965			
2000	5.031	48.787	44.554	8.467			
2100	5.065	49.033	44.761	8.971			
2200	5.111	49.270	44.961	9.480			
2300	5.171	49.499	45.153	9.994			
2400	5.249	49.720	45.339	10.515			
2500	5.345	49.936	45.519	11.044			
2600	5.461	50.148	45.693	11.584			
2700	5.600	50.357	45.862	12.137			
2800	5.762	50.563	46.026	12.705			
2900	5.949	50.769	46.186	13.291			
3000	6.159	50.974	46.342	13.896			
3100	6.394	51.180	46.495	14.5[illegible]			
3200	6.653	51.387	46.644	15.175			
3300	6.933	51.596	46.791	15.854			
3400	7.235	51.807	46.936	16.563			
3500	7.556	52.021	47.078	17.302			
3600	7.894	52.239	47.218	18.074			
3700	8.247	52.460	47.357	18.881			
3800	8.611	52.685	47.494	19.724			
3900	8.984	52.913	47.630	20.604			
4000	9.364	53.145	47.765	21.521			
4100	9.747	53.381	47.899	22.477			
4200	10.131	53.621	48.033	23.471			
4300	10.513	53.864	48.165	24.503			
4400	10.891	54.110	48.298	25.573			
4500	11.262	54.359	48.430	26.681			
4600	11.625	54.610	48.561	27.825			
4700	11.979	54.864	48.693	29.0[illegible]			
4800	12.320	55.120	48.824	30.22[illegible]			
4900	12.650	55.377	48.955	31.469			
5000	12.965	55.636	49.086	32.750			
5100	13.267	55.896	49.217	34.062			
5200	13.554	56.156	49.348	35.403			
5300	13.826	56.417	49.479	36.772			
5400	14.085	56.678	49.610	38.168			
5500	14.324	56.938	49.741	39.588			
5600	14.550	57.1[illegible]	49.871	41.032			
5700	14.762	57.458	50.002	42.498			
5800	14.959	57.716	50.133	43.984			
5900	14.141	57.974	50.264	45.489			
6000	15.309	58.230	50.394	47.011			

May 1962 RCF

STRONTIUM, MONATOMIC (Sr) (IDEAL GAS) gfw = 87.63

$\Delta H^o_{f0} = 39.139$ Kcal gfw^{-1}

$\Delta H^o_{f298.15} = 39.070$ Kcal gfw^{-1}

Ground State Configuration $^1S_0$

$S^o_{298.15} = 39.325$ cal degK^{-1} gfw^{-1}

$H^o_{298.15} - H^o_0 = 1.481$ kcal gfw^{-1}

Electronic levels and multiplicities

Source of Data

Energy levels from Moore[1].

Heat of Formation

Average of two vapor pressure determinations. Details by Barriault *et al*[2].

Heat Capacity and Entropy

Calculated using monatomic gas computer program.

References

1. Moore, C., Atomic Energy Levels, Vol, II Nat. Bur. Stds. (1952).

2. Barriault, R., *et al*, ASD-TR-61-260(May 1962), Pt. I.

STRONTIUM, MONATOMIC (Sr) (IDEAL GAS) GFW = 87.63

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T (cal/°K gfw)	$-(F^o_T - H^o_{298})/T$ (cal/°K gfw)	$H^o_T - H^o_{298}$ (Kcal/gfw)	ΔH^o_f (Kcal/gfw)	ΔF^o_f (Kcal/gfw)	Log K_p
298.15	± 0.000	± 0.002	± 0.002	± 0.000	± 0.500	± 0.560	± 0.410
862	± 0.000	± 0.002	± 0.002	± 0.000	± 0.500	± 1.000	± 0.250
862	± 0.000	± 0.002	± 0.002	± 0.000	± 0.500	± 1.000	± 0.250
1045	± 0.000	± 0.002	± 0.002	± 0.000	± 0.600	± 1.200	± 0.250
1045	± 0.000	± 0.002	± 0.002	± 0.000	± 0.750	± 1.200	± 0.250
1641	± 0.000	± 0.002	± 0.002	± 0.000	± 1.050	± 1.800	± 0.240
1641	± 0.000	± 0.002	± 0.002	± 0.000			
2000	± 0.000	± 0.002	± 0.002	± 0.000			
3000	± 0.001	± 0.002	± 0.002	± 0.001			
4000	± 0.002	± 0.003	± 0.003	± 0.002			
5000	± 0.003	± 0.003	± 0.003	± 0.004			
6000	± 0.003	± 0.003	± 0.003	± 0.006			

TANTALUM **REFERENCE STATE** **Ta**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ta from 0° to 3270°K, Liquid Ta from 3270° to 5706°K, Gaseous Ta from 5706° to 6000°K

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.358			
298.15	6.069	9.920	9.920	0.000			
300	6.074	9.958	9.920	0.011			
400	6.270	11.735	10.161	0.630			
500	6.382	13.147	10.622	1.263			
600	6.461	14.318	11.143	1.905			
700	6.525	15.319	11.670	2.554			
800	6.580	16.194	12.182	3.210			
900	6.630	16.972	12.672	3.870			
1000	6.673	17.673	13.137	4.536			
1100	6.720	18.311	13.579	5.205			
1200	6.769	18.898	13.998	5.880			
1300	6.824	19.442	14.396	6.559			
1400	6.883	19.950	14.775	7.244			
1500	6.949	20.428	15.136	7.937			
1600	7.022	20.878	15.481	8.636			
1700	7.102	21.306	15.811	9.342			
1800	7.190	21.715	16.128	10.057			
1900	7.289	22.106	16.432	10.780			
2000	7.398	22.483	16.725	11.515			
2100	7.521	22.847	17.008	12.261			
2200	[illegible]	23.200	17.282	13.019			
2300	7.812	23.543	17.547	13.793			
2400	7.995	23.880	17.803	14.583			
2500	8.215	24.212	18.053	15.397			
2600	8.491	24.539	18.296	16.230			
2700	8.851	24.866	18.534	17.097			
2800	9.309	25.195	18.765	18.004			
2900	9.873	25.531	18.993	18.962			
3000	10.532	25.877	19.216	19.982			
3100	11.266	26.234	19.437	21.071			
3200	12.065	26.604	19.655	22.237			
3270	12.663	26.871	19.807	23.102			
3270	8.500	28.920	19.807	29.802			
3300	8.500	28.998	19.890	30.057			
3400	8.500	29.252	20.161	30.907			
3500	8.500	29.498	20.425	31.757			
3600	8.500	29.738	20.680	32.607			
3700	8.500	29.970	20.928	33.457			
3800	8.500	30.197	21.169	34.307			
3900	8.500	30.418	21.403	35.157			
4000	8.500	30.633	21.631	36.007			
4100	8.500	30.843	21.853	36.857			
4200	8.500	31.048	22.070	37.707			
4300	8.500	31.248	22.281	38.557			
4400	8.500	31.443	22.487	39.407			
4500	8.500	31.634	22.688	40.257			
4600	8.500	31.821	22.885	41.107			
4700	8.500	32.004	23.077	41.957			
4800	8.500	32.183	23.265	42.807			
4900	8.500	32.358	23.448	43.657			
5000	8.500	32.530	23.628	44.507			
5100	8.500	32.698	23.805	45.35[illegible]			
5200	8.500	32.863	23.977	46.207			
5300	8.500	33.025	24.146	47.057			
5400	8.500	33.184	24.312	47.907			
5500	8.500	33.340	24.475	48.757			
5600	8.500	33.493	24.635	49.607			
5700	8.500	33.644	24.791	50.457			
5706.65	8.500	33.654	24.801	50.513			
5706.65	10.126	65.409	24.801	231.736			
5800	10.161	65.571	25.456	232.683			
5900	10.197	65.747	26.137	233.701			
6000	10.229	65.919	26.799	234.722			

15 March 1963 HLS

$0^{\circ}K$ to $3270^{\circ}K$	Crystal
$3270^{\circ}K$ to $5706^{\circ}K$	Liquid
$5706^{\circ}K$ to $6000^{\circ}K$	Ideal Monatomic Gas

$\Delta H^{o}_{f0} = 0$

$\Delta H^{o}_{s298.15} = 186.522$ Kcal gfw^{-1}

$T_m = 3270^{\circ}K$

$T_B = 5706.65^{\circ}K$

$H^{o}_{298} - H^{o}_{0} = 1.358$ Kcal gfw^{-1}

$\Delta H^{o}_{f298.15} = 0$

$S^{o}_{298.15} = 9.92$ cal degK^{-1} gfw^{-1}

$\Delta H_m = 6.700$ Kcal gfw^{-1}

$\Delta H_v = 181.223$ Kcal gfw^{-1}

$C^{o}_{p} = 6.31 + 0.40 \times 10^{-3}T - 0.32 \times 10^{5}T^{-2}$ cal degK^{-1} gfw^{-1} $\quad 298.15 \leq T \leq 950^{\circ}K$

C^{o}_{p} = smoothed curve approximating data of Lehman[1], Taylor and Finch[2], and Rasor and McClelland[3] for range 950° to 3270°K.

$C^{o}_{p} = 8.5$ cal degK^{-1} gfw^{-1} for liquid ($3270 \leq T \leq 5706^{\circ}K$) (Estd.)

Structure

Solid has B.C.C. A2 type structure, with no reported transitions to melting point.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Low temperature data from Kelley[4] and Sterrett and Wallace.[5] High temperature data is from Kelley[8] (298.15° to 950°K), and Lehman et al[1,2,3] for 950° to 3270°K. Liquid C^{o}_{p} is estimated.

Melting

Several values were available. The value listed by Stull and Sinke[6] was used. Heat of melting was an average of two estimates.

Heat of Sublimation

From Edwards, Johnston and Blackburn.[7]

References

1. Lehman, G. W., WADD TR 60-581 (1960).
2. Taylor, R. E. and R. A. Finch, NAA-SR-6034 (1961)
3. Rasor, N. and J. McClelland, WADC TR 56-400, AD118144 (1957).
4. Kelley, K. K., Bur. Mines Bull. 592 (1961).
5. Sterrett, K. F. and W. E. Wallace, J. Am. Chem. Soc. 80, 3177 (1958)
6. Stull, D. R. and G. C. Sinke, Thermodynamic Properties of the Elements (1956).
7. Edwards, J. W., H. L. Johnston, and P. E. Blackburn, J. Am. Chem. Soc. 73, 172 (1951).
8. Kelley, K. K., Bur. Mines, Bull. 584 (1960).

TANTALUM (Ta) (REFERENCE STATE) GFW = 180.95

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^{o}_{p} (cal/°K gfw)	S^{o}_{T} (cal/°K gfw)	$-(F^{o}_{T} - H^{o}_{298})/T$ (cal/°K gfw)	$H^{o}_{T} - H^{o}_{298}$ (Kcal/gfw)	ΔH^{o}_{f} (Kcal/gfw)	ΔF^{o}_{f} (Kcal/gfw)	Log K_p
298.15	± 0.050	± 0.040	± 0.040	± 0.000			
1000	± 0.100	± 0.103	± 0.065	± 0.038			
2000	± 0.500	± 0.345	± 0.136	± 0.418			
3000	± 1.000	± 0.639	± 0.249	± 1.168			
3270	± 1.000	± 0.725	± 0.285	± 1.438			
3270	± 2.000	± 1.031	± 0.285	± 2.438			
4000	± 2.000	± 1.434	± 0.459	± 3.898			
5000	± 2.000	± 1.880	± 0.700	± 5.898			

TABLE 234

TANTALUM — IDEAL MONATOMIC GAS — Ta

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ta from 0° to 3270°K, Liquid Ta from 3270° to 5706°K, Gaseous Ta from 5706° to 6000°K.

T, °K	cal/°K gfw			Kcal/gfw			Log K_p
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	
0	0.000	0.000	INFINITE	-1.482	186.398	186.398	INFINITE
298.15	4.985	44.243	44.243	0.000	186.522	176.289	-129.217
300	4.986	44.274	44.243	0.009	186.520	176.225	-128.374
400	5.081	45.719	44.440	0.512	186.404	172.810	-94.415
500	5.278	46.872	44.815	1.029	186.288	169.426	-74.052
600	5.541	47.857	45.241	1.570	186.187	166.063	-60.486
700	5.827	48.733	45.679	2.138	186.106	162.716	-50.800
800	6.110	49.530	46.111	2.735	186.047	159.379	-43.538
900	6.376	50.265	46.532	3.359	186.011	156.048	-37.892
1000	6.621	50.949	46.940	4.009	185.995	152.719	-33.375
1100	6.844	51.591	47.334	4.683	186.000	149.392	-29.680
1200	7.044	52.195	47.714	5.377	186.019	146.063	-26.600
1300	7.221	52.766	48.081	6.091	186.054	142.732	-23.994
1400	7.377	53.307	48.435	6.821	186.099	139.398	-21.760
1500	7.514	53.821	48.777	7.565	186.150	136.061	-19.823
1600	7.633	54.310	49.108	8.323	186.209	132.719	-18.128
1700	7.739	54.776	49.428	9.092	186.272	129.373	-16.631
1800	7.832	55.221	49.737	9.870	186.335	126.026	-15.301
1900	7.916	55.647	50.037	10.658	186.400	122.672	-14.110
2000	7.993	56.055	50.328	11.453	186.460	119.316	-13.038
2100	8.064	56.446	50.610	12.256	186.517	115.958	-12.067
2200	8.132	56.823	50.884	13.066	186.569	112.598	-11.185
2300	8.196	57.186	51.150	13.882	186.611	109.235	-10.379
2400	8.258	57.536	51.409	14.705	186.644	105.868	-9.640
2500	8.319	57.874	51.661	15.534	186.659	102.502	-8.960
2600	8.378	58.202	51.906	16.369	186.661	99.136	-8.333
2700	8.437	58.519	52.145	17.210	186.635	95.772	-7.752
2800	8.495	58.827	52.378	18.056	186.574	92.406	-7.212
2900	8.552	59.126	52.606	18.909	186.469	89.044	-6.710
3000	8.610	59.417	52.828	19.767	186.307	85.686	-6.242
3100	8.667	59.700	53.045	20.631	186.082	82.337	-5.804
3200	8.725	59.976	53.258	21.500	185.785	78.992	-5.395
3270	8.766	60.166	53.403	22.112	185.532	76.663	-5.124
3270	8.766	60.166	53.403	22.112	178.832	76.663	-5.124
3300	8.783	60.246	53.465	22.376	178.841	75.725	-5.015
3400	8.841	60.509	53.669	23.257	178.872	72.595	-4.666
3500	8.900	60.766	53.868	24.144	178.9[illegible]4	69.472	-4.338
3600	8.959	61.018	54.063	25.037	178.9[illegible]2	66.343	-4.027
3700	9.019	61.264	54.254	25.936	179.00[illegible]	63.216	-3.734
3800	9.079	61.505	54.442	26.841	179.056	60.085	-3.455
3900	9.139	61.742	54.626	27.752	179.117	56.952	-3.191
4000	9.200	61.974	54.807	28.668	179.183	53.818	-2.940
4100	9.261	62.202	54.984	29.592	179.257	50.685	-2.702
4200	9.322	62.426	55.159	30.521	179.336	47.548	-2.474
4300	9.383	62.646	55.330	31.456	179.421	44.411	-2.257
4400	9.444	62.862	55.499	32.397	179.512	41.269	-2.050
4500	9.504	63.075	55.665	33.345	179.610	38.126	-1.852
4600	9.564	63.285	55.829	34.298	179.713	34.980	-1.662
4700	9.623	63.491	55.989	35.258	179.823	31.836	-1.480
4800	9.680	63.694	56.148	36.223	179.938	28.684	-1.306
4900	9.737	63.894	56.304	37.194	180.059	25.528	-1.139
5000	9.792	64.092	56.458	38.170	180.185	22.372	-0.978
5100	9.846	64.286	56.609	39.152	180.317	19.222	-0.824
5200	9.897	64.478	56.759	[illegible].139	180.454	16.056	-0.675
5300	9.947	64.667	56.906	41.131	180.596	12.894	-0.532
5400	9.995	64.853	57.052	42.128	180.743	9.726	-0.394
5500	10.040	65.037	57.195	43.130	180.895	6.562	-0.261
5600	10.083	65.218	57.337	44.136	181.051	3.391	-0.132
5700	10.124	65.397	57.477	45.147	181.212	0.212	-0.008
5706.65	10.126	65.409	57.486	45.214	181.223	0.000	-0.000
5706.65	10.126	65.409	57.486	45.214	0.000	0.000	-0.000
5800	10.161	65.573	57.615	46.161			
5900	10.197	65.747	57.751	47.179			
6000	10.229	65.919	57.886	48.200			

15 March 1963 — HLS

ΔH^o_{f0} = 186.398 Kcal gfw^{-1}

Ground State Configuration $^4F_{1\frac{1}{2}}$

$H^o_{298}-H^o_0$ = 1.482 Kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 186.522 Kcal gfw^{-1}

$S^o_{298.15}$ = 44.243 cal degK^{-1}gfw^{-1}

Electronic Levels and Multiplicities

All levels listed by Moore[1]

Heat of Formation

The data of Edwards, Johnston, and Blackburn[2] were used. Other data analyzed included that of Langmuir and Malter,[3] Gebhardt, Seghezzi, and Keil,[4] and Fiske.[5]

Heat Capacity and Entropy

Calculated using the monatomic gas program.

References

1. Moore, C., National Bureau of Standards (U.S.) Circular 467, Vol. 3 (1958).
2. Edwards, J. W., H. L. Johnston, P. E. Blackburn, J. Am. Chem. Soc. 73, 172 (1951).
3. Langmuir, D. and L. Malter, Phys. Rev. 55, 748 (1939).
4. Gebhardt, E., H. Seghezzi, and H. Keil, Z. Metallkunde 53, 524 (1962).
5. Fiske, R., Phys. Rev. 61, 513 (1942).

TANTALUM, MONATOMIC (Ta) (IDEAL GAS) GFW = 180.95

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T (cal/°K gfw)	$-(F^o_T - H^o_{298})/T$ (cal/°K gfw)	$H^o_T - H^o_{298}$ (Kcal gfw)	ΔH^o_f (Kcal gfw)	ΔF^o_f (Kcal gfw)	Log K_p
298.15	± 0.000	± 0.002	± 0.002	± 0.000	± 3.000		
1000	± 0.001	± 0.002	± 0.003	± 0.000	3		
2000	± 0.002	± 0.003	± 0.003	± 0.001			
3000	± 0.006	± 0.004	± 0.003	± 0.004			
4000	± 0.012	± 0.006	± 0.004	± 0.012			
5000	± 0.016	± 0.009	± 0.004	± 0.026			
5706.65	± 0.014	± 0.011	± 0.005	± 0.038			
6000	± 0.013	± 0.012	± 0.005	± 0.041			

TABLE 235

TECHNETIUM — REFERENCE STATE — **Tc**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Tc from 0° to 2473°K, Liquid Tc from 2473° to 4840°K, Gaseous Tc from 4840° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.230			
298.15	5.800	8.000	8.000	0.000			
300	5.804	8.036	8.000	0.011			
400	6.004	9.733	8.230	0.601			
500	6.204	11.094	8.671	1.212			
600	6.404	12.243	9.173	1.842			
700	6.604	13.245	9.685	2.492			
800	6.804	14.140	10.187	3.163			
900	7.004	14.953	10.672	3.853			
1000	7.204	15.701	11.138	4.564			
1100	7.404	16.397	11.585	5.294			
1200	7.604	17.050	12.013	6.044			
1300	7.804	17.667	12.425	6.815			
1400	8.004	18.252	12.820	7.605			
1500	8.204	18.811	13.201	8.416			
1600	8.404	19.347	13.569	9.246			
1700	8.604	19.863	13.924	10.096			
1800	8.804	20.360	14.268	10.967			
1900	9.004	20.842	14.601	11.857			
2000	9.204	21.309	14.925	12.768			
2100	9.404	21.762	15.240	13.698			
2200	9.604	22.204	15.546	14.648			
2300	9.804	22.636	15.845	15.619			
2400	10.004	23.057	16.137	16.609			
2473	10.150	23.359	16.346	17.345			
2473	10.000	25.659	16.346	23.033			
2500	10.000	25.768	16.447	23.303			
2600	10.000	26.160	16.813	24.303			
2700	10.000	26.537	17.166	25.303			
2800	10.000	26.901	17.507	26.303			
2900	10.000	27.252	17.837	27.303			
3000	10.000	27.591	18.157	28.303			
3100	10.000	27.919	18.466	29.303			
3200	10.000	28.236	18.767	30.303			
3300	10.000	28.544	19.058	31.303			
3400	10.000	28.843	19.342	32.303			
3500	10.000	29.133	19.618	33.303			
3600	10.000	29.414	19.886	34.303			
3700	10.000	29.688	20.147	35.303			
3800	10.000	29.955	20.402	36.303			
3900	10.000	30.215	20.650	37.303			
4000	10.000	30.468	20.892	38.303			
4100	10.000	30.715	21.129	39.303			
4200	10.000	30.956	21.360	40.303			
4300	10.000	31.191	21.586	41.303			
4400	10.000	31.421	21.807	42.303			
4500	10.000	31.646	22.023	43.303			
4600	10.000	31.866	22.234	44.303			
4700	10.000	32.081	22.442	45.303			
4800	10.000	32.291	22.645	46.303			
4840.07	10.000	32.374	22.724	46.704			
4840.07	7.499	61.273	22.724	186.575			
4900	7.522	61.366	23.198	187.024			
5000	7.559	61.518	23.962	187.778			
5100	7.594	61.668	24.700	188.536			
5200	7.628	61.816	25.413	189.297			
5300	7.660	61.961	26.100	190.061			
5400	7.691	62.105	26.766	190.829			
5500	7.720	62.246	27.410	191.600			
5600	7.748	62.386	28.034	192.373			
5700	7.774	62.523	28.637	193.149			
5800	7.798	62.658	29.222	193.928			
5900	7.821	62.792	29.790	194.709			
6000	7.842	62.923	30.341	195.492			

TECHNETIUM (Tc) *(REFERENCE STATE)* *gfw = 99**

0^oK to 2473^oK	Crystal
2473^oK to 4840^oK	Liquid
4840^oK to 6000^oK	Ideal Monatomic Gas

$\Delta H^o_{f0} = 0$

$\Delta H^o_{f298.15} = 0$

$\Delta H_{s298.15} = 155.000$ kcal gfw^{-1}

$S^o_{298.15} = 8.000$ cal deg K^{-1}gfw^{-1}

$T_m = 2473^oK$

$\Delta H_m = 5.688$ kcal gfw^{-1}

$T_b = 4840^oK$

$\Delta H_v = 139.871$ kcal gfw^{-1}

$H^o_{298.15}-H^o_0 = 1.230$ kcal gfw^{-1}

$C^o_p = 5.200 + 2.000 \times 10^{-3}T$ cal deg K^{-1}gfw^{-1} cal deg K^{-1}gfw^{-1}

$298.15^oK \leq T \leq 2473^oK$

$C^o_p = 10.000$ cal deg K^{-1}gfw^{-1} $\quad 2473^oK \leq T \leq 4840^oK$

Structure

An h. c. p. (A3) type.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Brewer's[1] estimate of S^o_{298} adopted. Kelley's[2] high-temperature heat-capacity data adopted. Based on Brewer's[1] heat-content estimates. Liquid heat capacity estimated.

Melting and Vaporization

Heat of fusion estimated. Vapor-pressure data of Brewer[1] used in calculating b. p. Heat of vaporization calculated.

References

1. Brewer, L., Paper 3, Chemistry and Metallurgy of Miscellaneous Materials: Thermodynamics, Nat. Nucl. Energ. Ser. IV-19B, McGraw-Hill, N. Y. (1950).
2. Kelley, K. K., U. S. Bur. Mines, Bull. 584 (1960).

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* Isotope of longest known half-life.

TECHNETIUM (Tc) (REFERENCE STATE) GFW = 99

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T (cal/°K gfw)	$-(F^o_T - H^o_{298})/T$ (cal/°K gfw)	$H^o_T - H^o_{298}$ (kcal gfw)	ΔH_f (kcal gfw)	ΔF_f (kcal gfw)	Log K_p
298.15	± 0.100	± 0.500	± 0.500	± 0.000			
1000	± 0.500	± 0.740	± 0.600	± 0.140			
2000	± 1.000	± 1.260	± 0.600	± 0.890			
2473	± 1.250	± 1.500	± 0.810	± 1.420			
2473	± 0.500	± 1.900	± 0.920	± 2.420			
3000	± 1.550	± 2.100	± 0.920	± 2.960			
4000	± 3.550	± 2.830	± 1.110	± 4.510			
4840.07	± 5.230	± 3.670	± 1.700	± 8.200			
4840.07	± 0.001	± 0.003	± 0.003	± 0.002			
5000	± 0.001	± 0.003	± 0.003	± 0.002			
6000	± 0.001	± 0.003	± 0.003	± 0.003			

TABLE 236

TECHNETIUM

IDEAL MONATOMIC GAS

Tc

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Tc from 0° to 2473°K, Liquid Tc from 2473° to 4840°K, Gaseous Tc from 4840° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.481	154.749	154.749	INFINITE
298.15	4.970	43.250	43.250	0.000	155.000	144.490	-105.904
300	4.970	43.280	43.250	0.009	154.998	144.425	-105.208
400	4.999	44.713	43.445	0.507	154.976	140.214	-76.988
500	5.106	45.838	43.815	1.012	154.800	137.428	-60.067
600	5.328	46.767	44.233	1.532	154.690	133.964	-48.794
700	5.660	47.632	44.659	2.081	154.589	130.518	-40.748
800	6.060	48.413	45.080	2.667	154.504	127.086	-34.717
900	6.477	49.151	45.492	3.294	154.441	123.662	-30.028
1000	6.863	49.854	45.893	3.961	154.397	120.245	-26.278
1100	7.184	50.524	46.284	4.664	154.370	116.831	-23.211
1200	7.424	51.160	46.664	5.395	154.351	113.419	-20.655
1300	7.511	51.761	47.033	6.146	154.331	110.010	-18.493
1400	7.663	52.326	47.391	6.909	154.304	106.601	-16.640
1500	7.683	52.856	47.738	7.677	154.261	103.194	-15.035
1600	7.657	53.351	48.074	8.444	154.198	99.792	-13.630
1700	7.597	53.814	48.398	9.207	154.111	96.394	-12.392
1800	7.517	54.246	48.711	9.963	153.996	93.003	-11.292
1900	7.426	54.650	49.013	10.710	153.863	89.617	-10.308
2000	7.332	55.028	49.304	11.448	153.680	86.242	-9.424
2100	7.241	55.384	49.585	12.176	153.478	82.876	-8.625
2200	7.156	55.711	49.857	12.896	153.248	79.516	-7.899
2300	7.080	56.035	50.118	13.608	152.989	76.172	-7.238
2400	7.015	56.33[illegible]	50.371	14.313	152.704	72.838	-6.632
2473	6.974	56.543	50.549	14.923	152.478	70.416	-6.223
2473	6.974	56.543	50.549	14.823	146.790	70.416	-6.223
2500	6.961	56.620	50.615	15.011	146.798	69.580	-6.082
2600	6.918	56.812	50.812	15.705	146.402	66.499	-5.590
2700	6.887	57.15[illegible]	51.080	16.395	146.093	63.432	-5.134
2800	6.866	57.43[illegible]	51.302	17.083	145.780	60.374	-4.712
2900	6.856	57.643	51.516	17.769	145.466	57.331	-4.320
3000	6.854	57.876	51.724	18.454	145.151	54.299	-3.955
3100	6.860	58.101	51.926	19.140	144.937	51.274	-3.615
3200	6.874	58.317	52.13[illegible]	19.827	144.524	48.261	-3.296
3300	6.894	58.5[illegible]	52.314	20.515	144.217	45.255	-2.997
3400	6.920	58.737	52.50[illegible]	21.206	143.9[illegible]	42.263	-2.717
3500	6.950	58.938	52.681	[illegible].399	143.59[illegible]	39.280	-2.453
3600	6.984	59.134	52.857	22.596	143.22[illegible]	36.304	-2.204
3700	7.021	59.326	53.040	23.296	142.993	33.333	-1.969
3800	7.061	59.513	53.178	24.000	142.697	30.375	-1.747
3900	7.102	59.697	53.362	24.708	142.405	27.423	-1.537
4000	7.144	59.87[illegible]	53.52[illegible]	25.420	142.117	24.476	-1.337
4100	7.188	60.05[illegible]	53.660	26.137	141.934	21.541	-1.146
4200	7.231	60.22[illegible]	53.834	26.858	141.[illegible]	18.609	-0.968
4300	7.275	60.39[illegible]	[illegible].964	27.583	141.[illegible]	15.689	-0.797
4400	7.318	60.567	54.132	28.313	141.010	12.770	-0.634
4500	7.361	60.732	54.277	29.047	140.744	9.857	-0.477
4600	7.403	60.894	54.41[illegible]	29.785	140.482	6.949	-0.330
4700	7.444	61.054	54.558	30.528	140.22[illegible]	4.0[illegible]	-0.187
4800	7.464	61.211	54.695	31.274	13[illegible].97[illegible]	1.160	-0.053
4840.07	7.499	61.273	54.749	31.575	137.871	0.000	0.000
4840.07	7.499	61.273	54.749	31.575			
4900	7.522	61.366	54.832	32.024			
5000	7.559	61.518	54.962	3[illegible].778			
5100	7.594	61.668	55.092	33.536			
5200	7.628	61.816	55.22[illegible]	34.297			
5300	7.660	61.961	55.346	35.061			
5400	7.691	62.105	55.47[illegible]	35.829			
5500	7.723	62.246	55.5[illegible]2	36.600			
5600	7.748	62.386	55.712	37.373			
5700	7.774	62.52[illegible]	55.830	38.149			
5800	7.798	[illegible]	55.947	38.928			
5900	7.821	62.79[illegible]	56.062	39.709			
6000	7.847	62.9[illegible]	56.17[illegible]	40.41[illegible]			

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TECHNETIUM (Tc) (IDEAL MONATOMIC GAS) gfw = 99*

ΔH^{o}_{f0} = 154. 749 kcal gfw^{-1}

$\Delta H^{o}_{f298.15}$ = 155. 000 kcal gfw^{-1}

Ground State Configuration = $^{6}S_{2\frac{1}{2}}$

$S^{o}_{298.15}$ = 43. 250 cal deg K^{-1}gfw^{-1}

$H^{o}_{298.15}-H^{o}_{0}$ = 1. 481 kcal gfw^{-1}

Electronic Levels and Multiplicities

Spectroscopic energy levels from Moore.[1]

Heat of Formation

Estimate of Stull and Sinke[2] adopted. Based on vapor-pressure estimates of Brewer.[3]

Heat Capacity and Entropy

Calculated on monatomic-gas computer program.

References

1. Moore, C., Nat. Bur. Stds. (U. S.) Circ. 467, Vol. 3 (May 1958).
2. Stull, D. R. and G. C. Sinke, Advances in Chemistry, Ser. 18, Am. Chem. Soc., Washington, D. C. (1956).
3. Brewer, L., Paper 3, Chemistry and Metallurgy of Miscellaneous Materials: Thermodynamics, Natl. Nucl. Energ. Ser. IV-19B, McGraw-Hill, N. Y. (1950).

* Isotope of longest known half-life.

TECHNETIUM, MONATOMIC (Tc) (IDEAL GAS) GFW = 99

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw C^{o}_{p}	S^{o}_{T}	$-(F^{o}_{T}-H^{o}_{298})/T$	Kcal/gfw $H^{o}_{T}-H^{o}_{298}$	ΔH_f	ΔF_f	Log K_p
298.15	±0.000	± 0.002	± 0.002	± 0.000	± 5.000	± 5.150	±3.770
1000	±0.001	± 0.002	± 0.002	± 0.000	± 5.140	± 5.600	±1.220
2000	±0.001	± 0.003	± 0.003	± 0.001	± 5.890	± 6.630	±0.720
2473	±0.001	± 0.003	± 0.003	± 0.001	± 6.420	± 7.280	±0.640
2473	±0.001	± 0.003	± 0.003	± 0.001	± 7.420	± 7.280	±0.640
3000	±0X001	± 0.003	± 0.003	± 0.001	± 7.960	± 8.340	±0.610
4000	±0.001	± 0.003	± 0.003	± 0.002	± 9.510	±11.810	±0.650
4840.07	±0.001	± 0.003	± 0.003	± 0.002	±13.200	±14.600	±0.660
4840.07	±0.001	± 0.003	± 0.003	± 0.002			
5000	±0.001	± 0.003	± 0.003	± 0.002			
6000	±0.001	± 0.003	± 0.003	± 0.003			

THORIUM

REFERENCE STATE

Th

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Th from 0° to 2028°K, Liquid Th from 2028° to 5060°K, Gaseous Th from 5060° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.556			
298.15	6.532	12.760	12.760	0.000			
300	6.537	12.800	12.760	0.012			
400	6.792	14.716	13.020	0.679			
500	7.047	16.259	13.518	1.370			
600	7.302	17.566	14.086	2.088			
700	7.557	18.711	14.667	2.831			
800	7.812	19.737	15.238	3.599			
900	8.067	20.671	15.790	4.393			
1000	8.368	21.536	16.322	5.214			
1100	8.730	22.350	16.833	6.068			
1200	9.170	23.128	17.325	6.963			
1300	9.702	23.882	17.801	7.906			
1400	10.341	24.624	18.262	8.907			
1500	11.104	25.362	18.710	9.978			
1600	12.001	26.107	19.150	11.132			
1633	12.338	26.356	19.293	11.533			
1633	11.000	26.756	19.293	12.186			
1700	11.000	27.198	19.596	12.923			
1800	11.000	27.827	20.036	14.023			
1900	11.000	28.422	20.462	15.123			
2000	11.000	28.986	20.874	16.223			
2028	11.000	29.139	20.987	16.531			
2028	11.000	31.039	20.987	20.384			
2100	11.000	31.422	21.339	21.176			
2200	11.000	31.934	21.809	22.276			
2300	11.000	32.423	22.260	23.376			
2400	11.000	32.891	22.693	24.476			
2500	11.000	33.340	23.110	25.576			
2600	11.000	33.772	23.512	26.676			
2700	11.000	34.187	23.899	27.776			
2800	11.000	34.587	24.274	28.876			
2900	11.000	34.973	24.636	29.976			
3000	11.000	35.346	24.987	31.076			
3100	11.000	35.707	25.327	32.176			
3200	11.000	36.056	25.657	33.276			
3300	11.000	36.394	25.977	34.376			
3400	11.000	36.723	26.289	35.476			
3500	11.000	37.042	26.591	36.576			
3600	11.000	37.351	26.886	37.676			
3700	11.000	37.653	27.173	38.776			
3800	11.000	37.946	27.452	39.876			
3900	11.000	38.232	27.725	40.976			
4000	11.000	38.510	27.991	42.076			
4100	11.000	38.782	28.251	43.176			
4200	11.000	39.047	28.505	44.276			
4300	11.000	39.306	28.753	45.376			
4400	11.000	39.559	28.996	46.476			
4500	11.000	39.806	29.234	47.576			
4600	11.000	40.048	29.466	48.676			
4700	11.000	40.284	29.693	49.776			
4800	11.000	40.516	29.917	50.876			
4900	11.000	40.743	30.136	51.976			
5000	11.000	40.965	30.350	53.076			
5060.26	11.000	41.097	30.477	[illegible].739			
5060.26	9.340	65.357	30.477	176.504			
5100	9.356	65.430	30.749	176.875			
5200	9.394	65.612	31.417	177.812			
5300	9.430	65.792	32.065	178.753			
5400	9.464	65.968	32.691	179.698			
5500	9.496	66.142	33.297	180.646			
5600	9.525	66.314	33.886	181.597			
5700	9.552	66.482	34.456	182.551			
5800	9.575	66.649	35.010	183.507			
5900	9.596	66.813	35.548	184.466			
6000	9.613	66.974	36.070	185.426			

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RCF

THORIUM (Th) (REFERENCE STATE) gfw = 232.05

$0^\circ K$ to $2028^\circ K$	Crystal
$2028^\circ K$ to $5060^\circ K$	Liquid
$5060^\circ K$ to $6000^\circ K$	Ideal Monatomic Gas

$\Delta H^\circ_{f0} = 0$ $\Delta H^\circ_{f298.15} = 0$

$\Delta H^\circ_{s298.15} = 137.700$ kcal gfw^{-1} $S^\circ_{298.15} = 12.760$ cal deg K^{-1}gfw^{-1}

$T_t = 1633^\circ K$ $\Delta H_t = 0.653$ kcal gfw^{-1}

$T_m = 2028^\circ K$ $\Delta H_m = 3.853$ kcal gfw^{-1}

$T_b = 5060^\circ K$ $\Delta H_v = 122.765$ kcal gfw^{-1}

$H^\circ_{298.15} - H^\circ_0 = 1.556$ kcal gfw^{-1}

$C^\circ_p = 5.773 + 2.548 \times 10^{-3}T$ cal deg K^{-1}gfw^{-1} $298.15^\circ K \leq T \leq 800^\circ K$

$C^\circ_p = 5.553 + 4.928 \times 10^{-3}T - 4.703 \times 10^{-6}T^2$ cal deg K^{-1}gfw^{-1}

$800^\circ K \leq T \leq 1633^\circ K$

$C^\circ_p = 11.000$ cal deg K^{-1}gfw^{-1} $1633^\circ K \leq T \leq 2028^\circ K$

$C^\circ_p = 11.000$ cal deg K^{-1}gfw^{-1} $2028^\circ K \leq T \leq 5060^\circ K$

Structure

Two modifications f. c. c. (A1) and b. c. c. (A2) type.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Low-temperature data from Griffel and Shochdopole.[1] Wallace's[2] high-temperature heat-capacity data joined smoothly to low-temperature data Liquid heat capacity estimated.

Melting and Vaporization

Heat of fusion taken from estimate of Stull and Sinke.[3] Vapor-pressure data of Darnell et al[4] adopted. See volume 1, this study (section IVA29) for details.

References

1. Griffel, M and R. E. Shochdopole, J. Am Chem Soc. 75, 5250 (1953).
2. Wallace, D., Phys. Rev. 120, 84 (1956).
3. Stull, D. R. and G. C. Sinke, Advances in Chemistry, Ser. 18, Am. Chem. Soc., Washington, D. C. (1956).
4. Darnell, A. J., W. A. McCollum, and T. A. Milne, J. Phys Chem. 64, 341 (1960).

THORIUM (Th) (REFERENCE STATE) GFW = 232.05

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw C°_p	S°_T	$-(F^\circ_T - H^\circ_{298})/T$	Kcal/gfw $H^\circ_T - H^\circ_{298}$	ΔH°_f	ΔF_f	log K_p
298.15	± 0.050	± 0.200	± 0.200	± 0.000			
1000	± 0.150	± 0.260	± 0.220	± 0.040			
1633	± 0.250	± 0.360	± 0.260	± 0.160			
1633	± 1.000	± 0.480	± 0.260	± 0.360			
2028	± 1.000	± 0.700	± 0.320	± 0.760			
2028	± 0.600	± 1.190	± 0.320	± 1.760			
3000	± 2.800	± 1.860	± 0.720	± 3.410			
4000	± 5.000	± 2.980	± 1.150	± 7.310			
5060.26	± 7.300	± 4.420	± 1.690	±13.830			
5060.26	± 0.500	± 0.465	± 0.220	± 1.230			
6000	± 0.600	± 0.575	± 0.280	± 1.780			

THORIUM IDEAL MONATOMIC GAS **Th**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Th from 0° to 2028°K, Liquid Th from 2028° to 5060°K, Gaseous Th from 5060° to 6000°K.

T, °K	cal/°K gfw C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	Kcal/gfw $H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.481	137.775	137.775	INFINITE
298.15	4.969	45.426	45.426	0.000	137.700	127.961	-93.793
300	4.969	45.457	45.426	0.009	137.697	127.900	-93.171
400	4.982	46.888	45.621	0.506	137.527	124.660	-68.108
500	5.039	48.004	45.990	1.007	137.337	121.464	-53.089
600	5.171	48.934	46.405	1.517	137.129	118.309	-43.092
700	5.388	49.746	46.826	2.044	136.913	115.189	-35.962
800	5.679	50.484	47.237	2.597	136.698	112.101	-30.623
900	6.022	51.172	47.637	3.182	136.489	109.038	-26.477
1000	6.390	51.825	48.023	3.802	136.288	105.999	-23.165
1100	6.761	52.452	48.398	4.460	136.092	102.978	-20.459
1200	7.116	53.056	48.761	5.154	135.891	99.977	-18.207
1300	7.441	53.638	49.114	5.882	135.676	96.993	-16.305
1400	7.729	54.201	49.457	6.641	135.434	94.027	-14.678
1500	7.975	54.742	49.791	7.426	135.148	91.078	-13.269
1600	8.180	55.264	50.117	8.235	134.803	88.153	-12.041
1633	8.240	55.432	50.222	8.508	134.675	87.193	-11.669
1633	8.240	55.432	50.222	8.508	134.022	87.193	-11.669
1700	8.346	55.765	50.435	9.061	133.838	85.274	-10.962
1800	8.476	56.246	50.744	9.903	133.580	82.426	-10.007
1900	8.574	56.707	51.046	10.755	133.332	79.590	-9.155
2000	8.646	57.149	51.340	11.616	133.093	76.768	-8.388
2028	8.661	57.268	51.420	11.859	133.028	75.982	-8.188
2028	8.661	57.268	51.420	11.859	129.175	75.982	-8.188
2100	8.695	57.572	51.627	12.484	129.008	74.095	-7.711
2200	8.727	57.977	51.907	13.355	128.779	71.484	-7.101
2300	8.745	58.365	52.179	14.229	128.553	68.886	-6.545
2400	8.754	58.738	52.445	15.104	128.328	66.295	-6.037
2500	8.755	59.095	52.703	15.979	128.103	63.718	-5.570
2600	8.751	59.438	52.956	16.854	127.878	61.146	-5.140
2700	8.746	59.769	53.202	17.729	127.653	58.582	-4.742
2800	8.740	60.087	53.442	18.604	127.428	56.030	-4.373
2900	8.735	60.393	53.677	19.477	127.201	53.481	-4.030
3000	8.732	60.687	53.906	20.351	126.975	50.943	-3.711
3100	8.732	60.976	54.129	21.224	126.748	48.414	-3.413
3200	8.735	61.253	54.347	22.097	126.521	45.892	-3.134
3300	8.742	61.522	54.561	22.971	126.295	43.373	-2.872
3400	8.754	61.783	54.769	23.846	126.070	40.868	-2.627
3500	8.769	62.037	54.973	24.722	125.846	38.363	-2.395
3600	8.789	62.284	55.173	25.600	125.624	35.867	-2.177
3700	8.812	62.525	55.369	26.480	125.404	33.375	-1.971
3800	8.839	62.761	55.560	27.362	125.186	30.890	-1.776
3900	8.870	62.991	55.748	28.247	124.971	28.410	-1.592
4000	8.903	63.216	55.931	29.136	124.760	25.940	-1.417
4100	8.940	63.436	56.112	30.028	124.552	23.470	-1.251
4200	8.978	63.652	56.289	30.924	124.348	21.007	-1.093
4300	9.018	63.863	56.462	31.824	124.148	18.551	-0.943
4400	9.060	64.071	56.633	32.728	123.952	16.097	-0.799
4500	9.103	64.275	56.801	33.636	123.760	13.648	-0.663
4600	9.146	64.476	56.965	34.548	123.572	11.205	-0.532
4700	9.189	64.673	57.127	35.465	123.389	8.760	-0.407
4800	9.232	64.867	57.286	36.386	123.210	6.329	-0.288
4900	9.275	65.058	57.443	37.312	123.036	3.896	-0.174
5000	9.316	65.245	57.597	38.241	122.865	1.465	-0.064
5060.26	9.340	65.357	57.689	38.804	122.765	0.000	0.000
5060.26	9.340	65.357	57.689	38.804			
5100	9.356	65.430	57.749	39.175			
5200	9.394	65.612	57.899	40.112			
5300	9.430	65.792	58.046	41.053			
5400	9.464	65.968	58.191	41.998			
5500	9.496	66.142	58.334	42.946			
5600	9.525	66.314	58.475	43.897			
5700	9.552	66.482	58.614	44.851			
5800	9.575	66.649	58.751	45.807			
5900	9.596	66.813	58.886	46.766			
6000	9.613	66.974	59.020	47.726			

15 December 1962 RCF

THORIUM (Th) (IDEAL MONATOMIC GAS) gfw = 232.05

ΔH^o_{f0} = 137.775 kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 137.700 kcal gfw^{-1}

Ground State Configuration = $^3F_2$

$S^o_{298.15}$ = 45.426 cal deg K^{-1}gfw^{-1}

$H^o_{298.15}-H^o_0$ = 1.481 kcal gfw^{-1}

Electronic Levels and Multiplicities

Spectroscopic energy levels from Zalubas.[1]

Heat of Formation

Vapor-pressure data from Darnell *et al.*[2] ΔH^o_{298} derived from a Third Law calculation.

Heat Capacity and Entropy

Calculated from the monatomic-gas computer program. See volume 1, this study (section IVA29) for details.

References

1. Zalubas, R., J. Res. Natl. Bur. Stds. (U.S.) 63A, 275 (1959).
2. Darnell, A. J., W. A. McCollum, and T. A. Milne, J. Phys. Chem. 64, 341 (1960).

THORIUM, MONATOMIC (Th) (IDEAL GAS) GFW = 232.05

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T (cal/°K gfw)	$-(F^o_T - H^o_{298})/T$ (cal/°K gfw)	$H^o_T - H^o_{298}$ (Kcal/gfw)	ΔH^o_f (Kcal/gfw)	ΔF_f (Kcal/gfw)	Log K_p
298.15	± 0.010	± 0.005	± 0.005	± 0.000	± 1.000	± 1.060	± 0.780
1000	± 0.100	± 0.059	± 0.027	± 0.032	± 1.070	± 1.250	± 0.270
1633	± 0.160	± 0.120	± 0.050	± 0.120	± 0.280	± 1.510	± 0.200
1633	± 0.160	± 0.120	± 0.050	± 0.120	± 0.480	± 1.510	± 0.200
2028	± 0.200	± 0.160	± 0.070	± 0.180	± 0.940	± 1.790	± 0.190
2028	± 0.200	± 0.160	± 0.070	± 0.180	± 1.940	± 1.790	± 0.190
3000	± 0.300	± 0.260	± 0.120	± 0.430	± 3.840	± 3.520	± 0.260
4000	± 0.400	± 0.365	± 0.170	± 0.780	± 8.090	± 6.280	± 0.340
5060.26	± 0.500	± 0.465	± 0.220	± 1.230	±15.060	±10.660	± 0.460
5060.26	± 0.500	± 0.465	± 0.220	± 1.230			
6000	± 0.600	± 0.575	± 0.280	± 1.780			

TABLE 239

TITANIUM

REFERENCE STATE

Ti

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ti from 0° to 1950°K, Liquid Ti from 1950° to 3550°K, Gaseous Ti from 3550° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.150			
298.15	5.970	7.330	7.330	0.000			
300	5.980	7.367	7.330	0.011			
400	6.360	9.147	7.570	0.631			
500	6.620	10.595	8.035	1.280			
600	6.840	11.822	8.566	1.953			
700	7.020	12.890	9.109	2.647			
800	7.180	13.838	9.642	3.357			
900	7.330	14.693	10.157	4.082			
1000	7.470	15.472	10.650	4.822			
1100	7.600	16.190	11.121	5.576			
1155	7.667	16.563	11.372	5.996			
1155	7.667	17.385	11.372	6.946			
1200	7.720	17.679	11.603	7.292			
1300	7.840	18.302	12.094	8.070			
1400	7.950	18.887	12.559	8.860			
1500	8.060	19.439	12.999	9.660			
1600	8.160	19.963	13.418	10.471			
1700	8.260	20.460	13.818	11.292			
1800	8.360	20.935	14.200	12.123			
1900	8.460	21.390	14.567	12.964			
1950	8.510	21.610	14.745	13.388			
1950	8.000	23.507	14.745	17.088			
2000	8.000	23.710	14.966	17.489			
2100	8.000	24.101	15.392	18.289			
2200	8.000	24.473	15.796	19.089			
2300	8.000	24.829	16.181	19.889			
2400	8.000	24.169	16.549	20.689			
2500	8.000	25.496	16.900	21.489			
2600	8.000	25.809	17.237	22.289			
2700	8.000	26.111	17.560	23.089			
2800	8.000	26.402	17.871	23.889			
2900	8.000	26.683	18.170	24.689			
3000	8.000	26.954	18.458	25.489			
3100	8.000	27.217	18.736	26.289			
3200	8.000	27.470	19.005	27.089			
3300	8.000	27.717	19.266	27.889			
3400	8.000	27.955	19.518	28.689			
3500	8.000	28.187	19.762	29.489			
3550	8.000	28.303	19.881	29.889			
3550	8.068	57.162	19.881	132.346			
3600	8.137	57.275	20.400	132.751			
3700	8.274	57.500	21.400	133.571			
3800	8.408	57.723	22.353	134.405			
3900	8.539	57.943	23.262	135.253			
4000	8.666	58.160	24.132	136.113			
4100	8.790	58.376	24.965	136.986			
4200	8.910	58.589	25.763	137.871			
4300	9.026	58.800	26.529	138.768			
4400	9.137	59.009	27.265	139.676			
4500	9.244	59.216	27.972	140.595			
4600	9.346	59.420	28.654	141.524			
4700	9.443	59.622	29.310	142.464			
4800	9.535	59.822	29.944	·43.413			
4900	9.623	60.019	30.556	144.371			
5000	9.706	60.214	31.147	145.337			
5100	9.784	60.407	31.719	146.312			
5200	9.857	60.598	32.272	147.294			
5300	9.926	60.787	32.809	148.283			
5400	9.990	60.973	33.328	149.279			
5500	10.050	61.157	33.833	150.281			
5600	10.105	61.338	34.322	151.289			
5700	10.155	61.517	34.798	152.302			
5800	10.202	61.694	35.260	153.320			
5900	10.245	61.869	35.710	154.342			
6000	10.284	62.042	36.147	155.368			

May 1962 HLS

TITANIUM (Ti) (REFERENCE STATE) gfw = 47.90

0 °K to 1950 °K Crystal

1950 °K to 3550 °K Liquid

3550 °K to 6000 °K Ideal Monatomic Gas

$\Delta H^o_{f0} = 0$ $\Delta H^o_{f298.15} = 0$

$\Delta H^o_{s298.15} = 112.490$ Kcal gfw^{-1} $S^o_{298.15} = 7.330$ cal degK^{-1} gfw^{-1}

$T_t = 1155$ °K $\Delta H_t = 0.950$ Kcal gfw^{-1}

$T_m = 1950$ °K $\Delta H_m = 3.700$ Kcal gfw^{-1}

$T_b = 3550$ °K $\Delta H_v = 102.458$ Kcal gfw^{-1}

$H^o_{298.15} - H^o_0 = 1.150$ Kcal gfw^{-1}

Structure

Low temperature form (α - Ti) is h.c.p.; high temperature form (β - Ti) is b.c.c.

Heat of Formation

Zero by definition

Heat Capacity and Entropy

JANAF[1] tables results were accepted for this table.

Melting

Five values agreed with JANAF[1].

Vaporization

Three determinations had been made. Further details are given by Barriault *et al*[2].

References

1. JANAF Thermochemical Tables, Dow Chemical Co., Midland Mich. (1960).

2. Barriault, R., *et al*, ASD TR-61-260(May 1962), Pt. I.

TITANIUM (Ti) (REFERENCE STATE) GFW = 47.90

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T (cal/°K gfw)	$-(F^o_T - H^o_{298})/T$ (cal/°K gfw)	$H^o_T - H^o_{298}$ (Kcal/gfw)	ΔH^o_f (Kcal/gfw)	ΔF^o_f (Kcal/gfw)	Log K_p
298.15	±0.050	±0.020	±0.020	±0.000			
1000	±0.500	±0.346	±0.157	±0.189			
1155	±0.500	±0.418	±0.188	±0.266			
1155	±0.500	±0.504	±0.188	±0.366			
1950	±1.000	±0.896	±0.403	±0.962			
1950	±1.000	±1.152	±0.403	±1.462			
2000	±1.000	±1.177	±0.421	±1.512			
3000	±2.000	±1.785	±0.781	±3.012			
3550	±2.000	±2.121	±0.963	±4.112			
3550	±2.000	±0.003	±0.284	±1.002			
4000	±0.002	±0.003	±0.253	±1.002			
5000	±0.005	±0.003	±0.203	±1.003			
6000	±0.010	±0.003	±0.170	±1.004			

TABLE 240

TITANIUM — IDEAL MONATOMIC GAS — **Ti**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Ti from 0° to 1950°K, Liquid Ti from 1950° to 3550°K, Gaseous Ti from 3550° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.802	111.838	111.838	INFINITE
298.15	5.838	43.068	43.068	0.000	112.490	101.835	-74.643
300	5.831	43.104	43.068	0.011	112.490	101.769	-74.135
400	5.522	44.735	43.293	0.577	112.436	98.201	-53.652
500	5.344	45.946	43.707	1.120	112.330	94.654	-41.371
600	5.237	46.911	44.164	1.648	112.185	91.132	-33.193
700	5.170	47.712	44.615	2.168	112.011	87.636	-27.360
800	5.128	48.400	45.046	2.683	111.816	84.167	-22.992
900	5.104	49.002	43.453	3.194	111.602	80.724	-19.602
1000	5.095	49.539	45.835	3.704	111.372	77.305	-16.894
1100	5.106	50.025	46.194	4.214	111.128	73.909	-14.684
1155	5.118	50.275	46.383	4.496	110.990	72.052	-13.633
1155	5.118	50.275	46.383	4.496	110.040	72.052	-13.633
1200	5.132	50.471	46.532	4.726	109.974	70.574	-12.853
1300	5.176	50.883	46.851	5.241	109.661	67.306	-11.315
1400	5.237	51.269	47.153	5.762	109.392	64.057	-9.999
1500	5.313	51.633	47.440	6.289	109.119	60.829	-8.862
1600	5.403	51.978	47.713	6.825	108.844	57.619	-7.870
1700	5.506	52.309	47.974	7.370	108.568	54.425	-6.996
1800	5.616	52.627	48.223	7.926	108.293	51.248	-6.222
1900	5.736	52.934	48.463	8.494	108.020	48.087	-5.531
1950	5.799	53.084	48.580	8.782	107.884	46.512	-5.213
1950	5.799	53.084	48.580	8.782	104.184	46.512	-5.213
2000	5.863	53.231	48.694	9.074	104.075	45.033	-4.921
2100	5.995	53.520	48.917	9.667	103.868	42.087	-4.380
2200	6.131	53.802	49.133	10.273	103.674	39.150	-3.889
2300	6.269	54.078	49.342	10.893	103.494	36.222	-3.442
2400	6.411	54.348	49.545	11.527	103.328	33.299	-3.032
2500	6.553	54.612	49.742	12.175	103.176	30.386	-2.656
2600	6.698	54.872	49.934	12.837	103.038	27.475	-2.309
2700	6.843	55.127	50.122	13.514	102.915	24.571	-1.989
2800	6.988	55.379	50.305	14.206	102.807	21.672	-1.691
2900	7.134	55.627	50.485	14.912	102.713	18.776	-1.415
3000	7.281	55.871	50.660	15.633	102.634	15.883	-1.157
3100	7.427	56.112	50.832	16.368	102.569	12.994	-0.916
3200	7.571	56.350	51.001	17.118	102.519	10.102	-0.690
3300	7.715	56.585	51.166	17.882	102.493	7.218	-0.478
3400	7.857	56.818	51.329	18.661	102.462	4.328	-0.278
3500	7.998	57.048	51.489	19.454	102.[illegible]5	1.443	-0.090
3550	8.068	57.162	51.569	19.856	102.458	0.009	0.001
3550	8.068	57.162	51.569	19.856			
3600	8.137	57.275	51.647	20.261			
3700	8.274	57.500	51.802	21.081			
3800	8.408	57.722	51.955	21.915			
3900	8.539	57.942	52.106	22.763			
4000	8.666	58.160	52.254	23.623			
4100	8.790	58.376	52.401	24.496			
4200	8.910	58.589	52.546	25.381			
4300	9.026	58.800	52.689	26.277			
4400	9.137	59.009	52.830	27.186			
4500	9.244	59.215	52.970	28.105			
4600	9.346	59.419	53.108	29.034			
4700	9.443	59.621	53.244	29.974			
4800	9.535	59.821	53.379	30.923			
4900	9.623	60.019	53.513	31.881			
5000	9.706	60.214	53.645	32.847			
5100	9.784	60.407	53.775	33.822			
5200	9.857	60.598	53.905	34.804			
5300	9.926	60.786	54.033	35.793			
5400	9.990	60.972	54.160	36.789			
5500	10.050	61.156	54.285	37.791			
5600	10.105	61.338	54.509	38.798			
5700	10.156	61.517	54.533	39.812			
5800	10.202	61.694	54.654	40.829			
5900	10.245	61.869	54.775	41.852			
6000	10.284	62.041	54.895	42.878			

May 1962 — HLS

TITANIUM, MONATOMIC (Ti) (IDEAL GAS) gfw = 47.90

ΔH^o_{f0} = 111.838 Kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 112.490 Kcal gfw^{-1}

Ground State Configuration $^3F_2$

$S^o_{298.15}$ = 43.068 cal degK^{-1} gfw^{-1}

$H^o_{298.15} - H^o_0$ 1.802 Kcal gfw^{-1}

Electronic levels and multiplicities

Atomic energy levels from Moore[1].

Heat of Formation

Based on three vaporization determinations.

Heat Capacity and Entropy

A table had been calculated using the data from the present project.[2] It agreed well with JANAF[3]. In the interest of consistency, the latter data were accepted.

References

1. Moore, C., Atomic Energy Levels Vol. 1 Nat. Bur. Stds. (1949).
2. Barriault, R., et al, ASD TR-61-260 (May 1962), Pt. I.
3. JANAF Thermochemical Tables, Dow Chemical Co. (1960).

TITANIUM, MONATOMIC (Ti) (IDEAL GAS) GFW = 47.90

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw C^o_p	S^o_T	$-(F^o_T - H^o_{298})/T$	Kcal/gfw $H^o_T - H^o_{298}$	ΔH_f	ΔF_f	Log K_p
298.15	±0.000	±0.002	±0.003	±0.000	±1.000	±1.007	±0.738
1000	±0.001	±0.002	±0.003	±0.001	±1.190	±1.160	±0.253
1155	±0.001	±0.002	±0.003	±0.001	±1.267	±1.220	±0.230
1155	±0.001	±0.002	±0.003	±0.001	±1.367	±1.220	±0.230
1950	±0.001	±0.002	±0.003	±0.001	±1.963	±1.791	±0.200
1950	±0.001	±0.002	±0.003	±0.001	±2.463	±1.791	±0.200
2000	±0.001	±0.002	±0.003	±0.001	±2.513	±1.848	±0.201
3000	±0.001	±0.003	±0.003	±0.002	±4.014	±3.352	±0.244
3550	±0.002	±0.003	±0.003	±0.002	±5.114	±4.429	±0.272
3550	±0.002	±0.003	±0.003	±0.002			
4000	±0.002	±0.003	±0.002	±0.002			
5000	±0.005	±0.003	±0.003	±0.003			
6000	±0.010	±0.003	±0.004	±0.004			

TABLE 241

URANIUM REFERENCE STATE **U**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid U from 0° to 1406°K, Liquid U from 1406° to 4124°K, Gaseous U from 4124° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.521			
298.15	6.598	11.995	11.995	0.000			
300	6.608	12.036	11.995	0.012			
400	7.074	14.002	12.260	0.697			
500	7.569	15.632	12.776	1.428			
600	8.193	17.065	13.373	2.215			
700	8.983	18.385	13.996	3.072			
800	9.953	19.646	14.624	4.018			
900	11.109	20.883	15.251	5.069			
940	11.625	21.377	15.501	5.524			
940	10.150	22.106	15.501	6.209			
1000	10.150	22.734	15.916	6.818			
1048	10.150	23.210	16.239	7.305			
1048	9.150	24.278	16.239	8.425			
1100	9.150	24.722	16.630	8.901			
1200	9.150	25.518	17.338	9.816			
1300	9.150	26.250	17.996	10.731			
1400	9.150	26.928	18.610	11.646			
1406	9.150	26.967	18.645	11.701			
1406	9.150	30.310	18.645	16.401			
1500	9.150	30.902	19.395	17.261			
1600	9.150	31.493	20.133	18.176			
1700	9.150	32.048	20.818	19.091			
1800	9.150	32.571	21.456	20.006			
1900	9.150	33.065	22.054	20.921			
2000	9.150	33.535	22.617	21.836			
2100	9.150	33.981	23.147	22.751			
2200	9.150	34.407	23.650	23.666			
2300	9.150	34.813	24.126	24.581			
2400	9.150	35.203	24.580	25.496			
2500	9.150	35.576	25.012	26.411			
2600	9.150	35.935	25.425	27.326			
2700	9.150	36.281	25.821	28.241			
2800	9.150	36.613	26.201	29.156			
2900	9.150	36.934	26.565	30.071			
3000	9.150	37.245	26.916	30.986			
3100	9.150	37.545	27.254	31.901			
3200	9.150	37.835	27.580	32.816			
3300	9.150	38.117	27.895	33.731			
3400	9.150	38.390	28.200	34.646			
3500	9.150	38.655	28.495	35.561			
3600	9.150	38.913	28.781	36.476			
3700	9.150	39.164	29.058	37.391			
3800	9.150	39.408	29.327	38.306			
3900	9.150	39.645	29.589	39.221			
4000	9.150	39.877	29.843	40.136			
4100	9.150	40.103	30.090	41.051			
4123.63	9.150	40.156	30.148	41.267			
4123.63	10.288	66.079	30.147	148.168			
4200	10.327	66.268	30.803	148.955			
4300	10.377	66.512	31.630	149.990			
4400	10.425	66.751	32.426	151.031			
4500	10.472	66.985	33.191	152.075			
4600	10.515	67.216	33.928	[illegible]53.125			
4700	10.557	67.443	34.639	[illegible]4.178			
4800	10.595	67.665	35.325	155.236			
4900	10.630	67.884	35.986	156.297			
5000	10.662	68.099	36.627	157.362			
5100	10.690	68.311	37.246	158.430			
5200	10.715	68.519	37.846	159.500			
5300	10.735	68.723	38.426	160.572			
5400	10.751	68.924	38.989	161.647			
5500	10.763	69.121	39.535	162.722			
5600	10.770	69.315	40.065	163.799			
5700	10.773	69.506	40.580	164.876			
5800	10.771	69.693	41.081	165.954			
5900	10.765	69.877	41.567	167.030			
6000	10.755	70.058	42.040	168.106			

15 June 1963 MBP

URANIUM (U) (REFERENCE STATE) gfw = 238.07

0°K to 1406°K	Crystal
1406°K to 4124°K	Liquid
4124°K to 6000°K	Ideal Monatomic Gas

$\Delta H^\circ_{f0} = 0$ $\Delta H^\circ_{f298.15} = 0$

$\Delta H^\circ_{a298.15} = 117.064$ kcal gfw^{-1} $S^\circ_{298.15} = 11.995$ cal deg K^{-1}gfw^{-1}

$T_t = 940°K$ $\Delta H_t = 0.685$ kcal gfw^{-1}

$T_t = 1048°K$ $\Delta H_t = 1.120$ kcal gfw^{-1}

$T_m = 1406°K$ $\Delta H_m = 4.700$ kcal gfw^{-1}

$T_b = 4124°K$ $\Delta H_v = 106.901$ kcal gfw^{-1}

$H^\circ_{298.15} - H^\circ_0 = 1.521$ kcal gfw^{-1}

C°_p = smoothed data $298.15°K \leq T \leq 940°K$

$C^\circ_p = 10.150$ cal deg K^{-1}gfw^{-1} $940°K \leq T \leq 1048°K$

$C^\circ_p = 9.150$ cal degK^{-1}gfw^{-1} $1048°K \leq T \leq 4124°K$

Structure

Elemental uranium exists in three modifications (α, β, and γ) below melting point.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Low-temperature heat capacity by Flotow and Lohr.[1] High-temperature heat capacity from Ginnings and Corruccini.[2]

Melting and Vaporization

Heat of fusion based on work of Rauh and Thorn[3] Vapor-pressure data of Ackermann et al[4] and Rauh and Thorn[3] adopted.

References

1. Flotow, H. E. and H. R. Lohr, J. Phys. Chem. 64, 904 (1960).
2. Ginnings, D. C. and R. J Corruccini, J. Res. NBS 39, 309 (1947)
3. Rauh, E. G. and R. J. Thorn, J. Chem. Phys. 22, 1414 (1954)
4. Ackermann, R. J., E G. Rauh, and R J. Thorn, J Chem. Phys 37, 2693 (1962)

URANIUM (U) (REFERENCE STATE) GFW = 238.07

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal/gfw)	ΔH°_f (Kcal/gfw)	ΔF°_f (Kcal/gfw)	Log K_p
298.15	± 0.030	± 0.050	± 0.050	± 0.000			
350	± 0.030	± 0.055	± 0.050	± 0.002			
350	± 0.040	± 0.055	± 0.050	± 0.002			
600	± 0.040	± 0.076	± 0.057	± 0.012			
600	± 0.100	± 0.076	± 0.057	± 0.012			
900	± 0.100	± 0.117	± 0.071	± 0.042			
900	± 0.500	± 0.117	± 0.071	± 0.042			
939	± 0.500	± 0.138	± 0.073	± 0.061			
939	± 0.600	± 0.138	± 0.073	± 0.061			
940	± 0.600	± 0.139	± 0.073	± 0.062			
940	± 0.200	± 0.192	± 0.073	± 0.112			
1000	± 0.200	± 0.204	± 0.081	± 0.124			
1048	± 0.200	± 0.214	± 0.087	± 0.133			
1048	± 0.200	± 0.261	± 0.087	± 0.183			
1406	± 0.200	± 0.320	± 0.139	± 0.255			
1406	± 0.400	± 0.462	± 0.139	± 0.455			
2000	± 0.400	± 0.603	± 0.257	± 0.692			
2000	± 1.000	± 0.603	± 0.257	± 0.692			
3000	± 1.000	± 1.009	± 0.445	± 1.692			
3000	± 1.500	± 1.009	± 0.445	± 1.692			
4000	± 1.500	± 1.440	± 0.642	± 3.192			
4123.63	± 1.500	± 1.486	± 0.667	± 3.377			
4123.63	± 2.000	± 1.534	± 0.667	± 3.577			
5000	± 2.000	± 1.920	± 0.854	± 5.330			
6000	± 2.000	± 2.284	± 1.062	± 7.330			

URANIUM

IDEAL MONATOMIC GAS

U

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid U from 0° to 1406°K, Liquid U from 1406° to 4124°K, Gaseous U from 4124° to 6000°K.

T, °K	C_p° (cal/°K g/w)	S_T° (cal/°K g/w)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K g/w)	$H_T^\circ - H_{298}^\circ$ (Kcal/g/w)	ΔH_f° (Kcal/g/w)	ΔF_f° (Kcal/g/w)	Log K_p
0	0.000	0.000	INFINITE	-1.553	117.032	117.032	INFINITE
298.15	5.663	47.726	47.726	0.000	117.064	106.411	-77.997
300	5.666	47.761	47.726	0.010	117.062	106.345	-77.468
400	5.724	49.404	47.950	0.582	116.949	102.788	-56.158
500	5.665	50.676	48.373	1.152	116.788	99.266	-43.387
600	5.593	51.702	46.845	1.714	116.563	95.781	-34.887
700	5.559	52.561	49.316	2.271	116.263	92.340	-28.828
800	5.580	53.304	49.769	2.828	115.874	88.948	-24.298
900	5.660	53.965	50.199	3.389	115.384	85.611	-20.788
940	5.707	54.212	50.365	3.617	115.157	84.292	-19.597
940	5.707	54.212	50.365	3.617	114.472	84.292	-19.597
1000	5.792	54.568	50.606	3.962	114.208	82.374	-18.002
1048	5.873	54.841	50.794	4.242	114.001	80.850	-16.860
1048	5.873	54.841	50.794	4.242	112.881	80.850	-16.860
1100	5.970	55.128	50.992	4.549	112.712	79.266	-15.748
1200	6.182	55.656	51.359	5.157	112.405	76.239	-13.884
1300	6.420	56.160	51.709	5.787	112.120	73.237	-12.312
1400	6.674	56.645	52.044	6.441	111.859	70.256	-10.967
1406	6.689	56.674	52.064	6.481	111.844	70.077	-10.892
1406	6.689	56.674	52.064	6.481	107.144	70.077	-10.892
1500	6.936	57.115	52.367	7.122	106.925	67.606	-9.850
1600	7.200	57.571	52.678	7.829	106.717	64.992	-8.877
1700	7.460	58.015	52.979	8.562	106.535	62.390	-8.020
1800	7.712	58.449	53.271	9.320	106.378	59.797	-7.260
1900	7.951	58.872	53.555	10.104	106.247	57.213	-6.581
2000	8.176	59.286	53.831	10.910	106.138	54.636	-5.970
2100	8.385	59.690	54.100	11.738	106.051	52.062	-5.418
2200	8.577	60.084	54.363	12.587	105.985	49.495	-4.917
2300	8.753	60.470	54.620	13.453	105.936	46.927	-4.459
2400	8.912	60.846	54.872	14.337	105.905	44.363	-4.040
2500	9.056	61.212	55.118	15.235	105.888	41.798	-3.654
2600	9.185	61.570	55.360	16.147	105.885	39.234	-3.298
2700	9.302	61.919	55.596	17.072	105.895	36.671	-2.968
2800	9.407	62.259	55.828	18.007	105.915	34.108	-2.662
2900	9.502	62.591	56.056	18.953	105.946	31.541	-2.377
3000	9.589	62.915	56.279	19.907	105.985	28.976	-2.111
3100	9.669	63.230	56.498	20.870	106.033	26.408	-1.862
3200	9.742	63.538	56.713	21.841	106.089	23.838	-1.628
3300	9.811	63.839	56.925	22.819	106.152	21.266	-1.408
3400	9.877	64.133	57.132	23.803	106.221	18.694	-1.202
3500	9.939	64.420	57.336	24.794	106.297	16.119	-1.006
3600	9.999	64.701	57.537	25.791	106.379	13.542	-0.822
3700	10.057	64.976	57.735	26.794	106.467	10.961	-0.647
3800	10.114	65.245	57.929	27.802	106.560	8.378	-0.482
3900	10.169	65.508	58.120	28.816	106.659	5.795	-0.325
4000	10.223	65.767	58.308	29.836	106.764	3.206	-0.175
4100	10.276	66.020	58.493	30.861	106.874	0.613	-0.033
4123.63	10.288	66.079	58.536	31.104	106.901	0.003	-0.000
4123.63	10.288	66.079	58.536	31.104			
4200	10.327	66.268	58.675	31.891			
4300	10.377	66.512	58.854	32.926			
4400	10.425	66.751	59.031	33.967			
4500	10.472	66.985	59.205	35.011			
4600	10.515	67.216	59.377	36.[illegible]			
4700	10.557	67.443	59.546	37.114			
4800	10.595	67.665	59.713	38.172			
4900	10.630	67.884	59.877	39.233			
5000	10.662	68.099	60.040	40.298			
5100	10.690	68.311	60.200	41.366			
5200	10.715	68.519	60.358	42.436			
5300	10.735	68.723	60.514	43.508			
5400	10.751	68.924	60.668	44.583			
5500	10.763	69.[illegible]21	60.819	45.658			
5600	10.770	69.315	60.969	46.735			
5700	10.773	69.506	61.118	47.812			
5800	10.771	69.693	61.264	48.890			
5900	10.765	69.877	61.408	49.966			
6000	10.755	70.058	61.551	51.042			

15 June 1963

MBP

URANIUM (U) (IDEAL MONATOMIC GAS) gfw = 238.07

ΔH^o_{f0} = 117.032 kcal gfw^{-1} $\Delta H^o_{f298.15}$ = 117.064 kcal gfw^{-1}

$H^o_{298.15} - H^o_0$ = 1.553 kcal gfw^{-1} $S^o_{298.15}$ = 47.726 cal deg K^{-1}gfw^{-1}

Electronic Levels and Multiplicities

Spectroscopic energy levels from Blaise.[1]

Heat of Formation

Vapor-pressure data from Rauh and Thorn[2] adopted to calculate $\Delta H_{f298.15}$.

Heat Capacity and Entropy

Calculated on monatomic-gas computer program.

References

1. Blaise, J., unpublished work, provided by C. M Moore (Sitterly), NBS (1963).
2. Rauh, E. G. and R. J. Thorn, J. Chem. Phys. 22, 1414 (1954)

URANIUM, MONATOMIC (U) (IDEAL GAS) GFW = 238.07

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T (cal/°K gfw)	$-(F^o_T - H^o_{298})/T$ (cal/°K gfw)	$H^o_T - H^o_{298}$ (Kcal/gfw)	ΔH^o_f (Kcal/gfw)	ΔF^o_f (Kcal/gfw)	Log K_p
298.15	± .000	± .002	± .002	± .000			
940	± .000	± .002	± .002	± .000			
1000	± .000	± .002	± .002	± .000			
1048	± .000	± .002	± .002	± .000			
1406	± .001	± .002	± .002	± .000			
2000	± .001	± .003	± .003	± .001			
3000	± .002	± .003	± .003	± .002			
4000	± .002	± .003	± .003	± .003			
5000	± .002	± .003	± .003	± .004			
6000	± .002	± .004	± .003	± .005			

TABLE 243

VANADIUM

REFERENCE STATE

V

Reference State for Calculating ΔH°_f, ΔF°_f, and Log K_p: Solid V from 0° to 2190°K, Liquid V from 2190° to 3648°K, Gaseous V from 3648° to 6000°K.

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal/gfw)	ΔH°_f (Kcal/gfw)	ΔF°_f (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.122			
298.15	5.894	6.880	6.880	0.000			
300	5.896	6.916	6.880	0.011			
400	6.057	8.633	7.113	0.608			
500	6.270	10.007	7.559	1.224			
600	6.504	11.170	8.066	1.863			
700	6.747	12.191	8.584	2.525			
800	6.995	13.108	9.093	3.212			
900	7.247	13.946	9.586	3.924			
1000	7.500	14.723	10.062	4.661			
1100	7.755	15.450	10.519	5.424			
1200	8.010	16.135	10.958	6.212			
1300	8.266	16.787	11.382	7.026			
1400	8.522	17.409	11.790	7.866			
1500	8.779	18.005	12.185	8.731			
1600	9.036	18.580	12.567	9.621			
1700	9.293	19.136	12.937	10.538			
1800	9.550	19.674	13.296	11.480			
1900	9.808	20.197	13.646	12.448			
2000	[illegible].065	20.707	13.986	13.441			
2100	10.323	21.204	14.318	14.461			
2190	10.554	21.642	14.610	15.400			
2190	9.500	23.560	14.610	19.600			
2200	9.500	23.603	14.651	19.695			
2300	9.500	24.026	15.049	20.645			
2400	9.500	24.430	15.432	21.595			
2500	9.500	24.818	15.800	22.545			
2600	9.500	25.190	16.154	23.495			
2700	9.500	25.549	16.495	24.445			
2800	9.500	25.894	16.825	25.395			
2900	9.500	26.228	17.143	26.345			
3000	9.500	26.550	17.451	27.295			
3100	9.500	26.861	17.750	28.245			
3200	9.500	27.163	18.039	29.1[illegible]			
3300	9.500	27.455	18.320	30.145			
3400	9.500	27.739	18.593	31.095			
3500	9.500	28.014	18.858	32.045			
3600	9.500	28.282	19.117	32.995			
3647.68	9.500	28.407	19.237	33.448			
3647.68	6.890	58.528	19.237	143.322			
3700	6.950	58.627	19.794	143.683			
3800	7.068	58.814	20.818	144.384			
3900	7.188	58.999	21.795	145.097			
4000	7.311	59.183	22.728	145.822			
4100	7.435	59.365	23.619	146.559			
4200	7.560	59.546	24.472	147.309			
4300	7.685	59.725	25.290	148.071			
4400	7.810	59.903	26.074	148.846			
4500	7.935	60.080	26.828	149.633			
4600	8.058	60.256	27.553	150.433			
4700	8.180	60.430	28.251	151.[illegible]			
4800	8.300	60.604	28.923	152.069			
4900	8.419	60.776	29.571	152.905			
5000	8.534	60.947	30.197	153.753			
5100	8.648	61.118	30.801	154.612			
5200	8.758	61.287	31.386	155.482			
5300	8.866	61.454	31.952	156.363			
5400	8.970	61.621	32.499	157.255			
5500	9.071	61.787	33.031	158.157			
5600	9.169	61.951	33.546	159.069			
5700	9.264	62.114	34.045	159.991			
5800	9.354	62.276	34.530	160.922			
5900	9.442	62.437	35.003	161.862			
6000	9.526	62.596	35.461	162.810			

15 March 1963

HLS

$0^\circ K$ to $2190^\circ K$	Crystal
$2190^\circ K$ to $3648^\circ K$	Liquid
$3648^\circ K$ to $6000^\circ K$	Ideal Monatomic Gas

$\Delta H^\circ_{f0} = 0$

$\Delta H^\circ_{f298.15} = 0$

$\Delta H^\circ_{s298.15} = 123.010$ Kcal gfw^{-1}

$S^\circ_{298.15} = 6.88 \pm .05$ cal $degK^{-1}$ gfw^{-1}

$T_m = 2190^\circ K$

$\Delta H_m = 4.2$ Kcal gfw^{-1}

$T_b = 3647.68^\circ K$

$\Delta H_v = 109.874$ Kcal gfw^{-1}

$H^\circ_{298.15} - H^\circ_0 = 1.122$ Kcal gfw^{-1}

$C^\circ_p = 4.90 + 2.58 \times 10^{-3}T + 0.20 \times 10^5 T^{-2}$ cal deg^{-1} gfw^{-1} $298.15^\circ K \leq T \leq 2190^\circ K$

$C^\circ_p = 9.5 \pm 1$ cal $deg^{-1} gfw^{-1}$ for liquid ($2190^\circ K \leq T \leq 3648^\circ K$) (Estd)

Structure

Solid has b. c. c. A2 type structure to melting point.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Low temperature data by Anderson,[1] Stull and Sinke,[2] and Bieganski and Stalinski[3] High temperature data from Kelley.[4] Liquid heat capacity estimated by Kelley[4]

Melting

Estimated by Stull and Sinke.[2]

Heat of Sublimation

Recalculation of vapor pressure data of Edwards et al[5]

References

1. Anderson, C. T., J. Am. Chem. Soc. 52, 2296 (1930).
2. Stull, D. R. and G. Sinke, Thermodynamic Properties of the Elements (1956).
3. Bieganski, Z. and B. Stalinski, Bull.de l'acad. Pol. des sci.,Serie des science Chim. 9, 367 (1961)
4. Kelley, K. K., Bur. Mines, Bull. 584 (1960)
5. Edwards, J., H. Johnston and P. Blackburn, J. Am. Chem. Soc. 73, 4727 (1951)

VANADIUM (V) (REFERENCE STATE) GFW = 50.95

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal/gfw)	ΔH°_f (Kcal/gfw)	ΔF°_f (Kcal/gfw)	Log K_p
298.15	±0.050	±0.050	±0.050	±0.000			
1000	±0.200	±0.214	±0.104	±0.110			
2000	±1.000	±0.583	±0.228	±0.710			
2190	±1.000	±0.674	±0.263	±0.900			
2190	±2.000	±1.131	±0.263	±1.900			
3000	±2.000	±1.760	±0.587	±3.520			
3647.68	±2.000	±2.125	±0.814	±4.720			
3647.68	±0.001	±0.003					
4000	±0.001	±0.003					
5000	±0.002	±0.003					
6000	±0.003	±0.004					

TABLE 244

VANADIUM — IDEAL MONATOMIC GAS — V

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid V from 0° to 2190°K, Liquid V from 2190° to 3648°K, Gaseous V from 3648° to 6000°K.

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.890	122.242	122.242	INFINITE
298.15	6.217	43.546	43.546	0.000	123.010	112.078	-82.152
300	6.209	43.584	43.546	0.011	123.010	112.010	-81.595
400	5.891	45.321	43.785	0.615	123.017	108.341	-59.192
500	5.783	46.621	44.227	1.197	122.983	104.676	-45.752
600	5.804	47.676	44.717	1.775	122.922	101.019	-36.795
700	5.875	48.576	45.205	2.359	122.844	97.375	-30.400
800	5.949	49.365	45.677	2.951	122.749	93.743	-25.608
900	6.003	50.069	46.127	3.548	122.634	90.123	-21.884
000	6.032	50.704	46.553	4.150	122.499	86.519	-18.908
1100	6.038	51.279	46.957	4.754	122.340	82.928	-16.476
1200	6.026	51.804	47.339	5.357	122.155	79.352	-14.451
1300	6.003	52.285	47.702	5.959	121.943	75.795	-12.742
1400	5.974	52.729	48.045	6.558	121.702	72.253	-11.279
1500	5.943	53.140	48.371	7.154	121.433	68.731	-10.014
1600	5.913	53.523	48.681	7.746	121.135	65.227	-8.909
1700	5.887	53.881	48.977	8.336	120.808	61.742	-7.937
1800	5.867	54.216	49.259	8.924	120.454	58.277	-7.075
1900	5.853	54.533	49.528	9.510	120.072	54.834	-6.307
2000	5.846	54.833	49.786	10.095	119.664	51.410	-5.618
2100	5.848	55.119	50.033	10.680	119.229	48.008	-4.996
2190	5.857	55.364	50.247	11.206	118.816	44.965	-4.487
2190	5.857	55.364	50.247	11.206	114.616	44.965	-4.487
2200	5.858	55.391	50.270	11.265	114.580	44.647	-4.435
2300	5.877	55.652	50.499	11.851	114.216	41.476	-3.941
2400	5.904	55.902	50.719	12.440	113.855	38.322	-3.490
2500	5.940	56.144	50.931	13.033	113.498	35.183	-3.076
2600	5.985	56.378	51.136	13.629	113.144	32.057	-2.694
2700	6.038	56.605	51.334	14.230	112.795	28.944	-2.343
2800	6.099	56.825	51.526	14.837	112.452	25.846	-2.017
2900	6.168	57.040	51.713	15.450	112.115	22.757	-1.715
3000	6.245	57.251	51.894	16.070	111.785	19.681	-1.434
3100	6.328	57.457	52.070	16.699	111.464	16.617	-1.171
3200	6.418	57.659	52.242	17.336	111.151	13.561	-0.926
3300	6.515	57.858	52.409	17.983	110.848	10.517	-0.696
3400	6.617	58.054	52.572	18.639	110.554	7.481	-0.481
3500	6.723	58.248	52.731	19.306	110.271	4.453	-0.278
3600	6.835	58.439	52.887	19.984	109.999	1.437	-0.087
3647.68	6.889	58.529	52.960	20.311	109.873	-0.002	0.000
3647.68	6.889	58.529	52.960	20.311			
3700	6.950	58.627	53.040	20.673			
3800	7.068	58.814	53.189	21.374			
3900	7.188	58.999	53.336	22.087			
4000	7.311	59.183	53.480	22.812			
4100	7.435	59.365	53.621	23.549			
4200	7.560	59.546	53.760	24.299			
4300	7.685	59.725	53.897	25.061			
4400	7.810	59.903	54.031	25.836			
4500	7.935	60.080	54.164	26.623			
4600	8.058	60.256	54.294	27.423			
4700	8.180	60.430	54.423	28.235			
4800	8.300	60.604	54.550	29.059			
4900	8.419	60.776	54.675	29.895			
5000	8.534	60.947	54.799	30.743			
5100	8.648	61.118	54.921	31.602			
5200	8.758	61.287	55.042	32.472			
5300	8.866	61.454	55.161	33.353			
5400	8.970	61.621	55.279	34.245			
5500	9.071	61.787	55.396	35.147			
5600	9.169	61.951	55.512	36.059			
5700	9.264	62.114	55.626	36.981			
5800	9.354	62.276	55.739	37.912			
5900	9.442	62.437	55.852	38.852			
6000	9.526	62.596	55.963	39.800			

15 March 1963 — HLS

ΔH°_{f0} = 122.242 Kcal gfw^{-1}

Ground State Configuration $^4F_{1\frac{1}{2}}$

$H^\circ_{298.15}-H^\circ_0$ = 1.890 Kcal gfw^{-1}

$\Delta H^\circ_{f298.15}$ = 123.010 ± 4.0 Kcal gfw^{-1}

$S^\circ_{298.15}$ = 43.546 cal degK^{-1} gfw^{-1}

Electronic Levels and Multiplicities

All energy levels listed by Moore[1] were used.

Heat of Formation

The vapor pressure data of Edwards, Johnston and Blackburn[2] were used

Heat Capacity and Entropy

Calculated using the monatomic gas program.

References

1. Moore, C., Nat. Bur. Std. (U S.), Circ. 467, Vol. 1 (1949).
2. Edwards, J., H. Johnston and P. Blackburn, J. Am. Chem. Soc. 73, 4727 (1951)

VANADIUM, MONATOMIC (V) (IDEAL GAS) GFW = 50.95

SUMMARY OF UNCERTAINTY ESTIMATES

T,°K	C°_p (cal/°K gfw)	S°_T (cal/°K gfw)	$-(F^\circ_T - H^\circ_{298})/T$ (cal/°K gfw)	$H^\circ_T - H^\circ_{298}$ (Kcal/gfw)	ΔH°_f (Kcal/gfw)	ΔF°_f (Kcal/gfw)	Log K_p
298.15	± 0.000	± 0.002	± 0.003	± 0.000	± 4.000		
1000	± 0.000	± 0.002	± 0.003	± 0.000			
2000	± 0.000	± 0.003	± 0.003	± 0.001			
3000	± 0.001	± 0.003	± 0.003	± 0.001			
3647.68	± 0.001	± 0.003	± 0.003	± 0.002			
4000	± 0.001	± 0.003	± 0.003	± 0.002			
5000	± 0.002	± 0.003	± 0.003	± 0.003			
6000	± 0.003	± 0.004	± 0.003	± 0.005			

TABLE 245

TUNGSTEN

REFERENCE STATE

W

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid W from 0° to 3650°K, Liquid W from 3650° to 5891°K, Gaseous W from 5891° to 6000°K.

T, °K	cal/°K gfw. C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	Kcal/gfw. $H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.195			
298.15	5.800	7.830	7.830	0.000			
300	5.810	7.866	7.830	0.011			
400	5.960	9.580	8.082	0.599			
500	6.040	10.901	8.501	1.200			
600	6.110	12.027	9.015	1.807			
700	6.180	12.955	9.496	2.421			
800	6.240	13.803	9.999	3.043			
900	6.300	14.523	10.444	3.671			
1000	6.360	15.209	10.906	4.303			
1100	6.430	15.799	11.305	4.943			
1200	6.520	16.382	11.724	5.589			
1300	6.650	16.888	12.082	6.248			
1400	6.800	17.386	12.442	6.921			
1500	6.950	17.860	12.788	7.608			
1600	7.100	18.313	13.119	8.311			
1700	7.250	18.748	13.437	9.028			
1800	7.400	19.167	13.744	9.761			
1900	7.550	19.571	14.040	10.508			
2000	7.700	19.962	14.326	11.271			
2100	7.850	20.342	14.605	12.048			
2200	8.000	20.710	14.873	12.841			
2300	8.150	21.069	15.135	13.648			
2400	8.300	21.419	15.389	14.471			
2500	[illegible].450	21.761	15.638	15.308			
2600	8.600	22.095	15.879	16.161			
2700	8.750	22.423	16.116	17.028			
2800	8.900	22.744	16.347	17.911			
2900	9.050	23.059	16.573	18.808			
3000	9.200	23.368	16.794	19.721			
3100	9.350	23.672	17.011	20.648			
3200	9.500	23.971	17.224	21.591			
3300	9.650	24.266	17.433	22.548			
3400	9.800	24.556	17.638	23.521			
3500	9.950	24.842	17.840	24.508			
3600	10.100	25.125	18.039	25.511			
3650	10.175	25.265	18.137	26.017			
3650	10.000	27.565	18.137	34.412			
3700	10.000	27.701	18.265	34.[illegible]12			
3800	10.000	27.968	18.517	35.912			
3900	10.000	28.227	18.762	36.912			
4000	10.000	28.481	19.003	37.912			
4100	10.000	28.727	19.236	38.912			
4200	10.000	28.968	19.465	39.912			
4300	10.000	29.204	19.690	40.912			
4400	10.000	29.434	19.909	41.912			
4500	10.000	29.658	20.122	42.912			
4600	10.000	29.878	20.332	43.912			
4700	10.000	30.093	20.537	44.912			
4800	10.000	30.304	20.739	45.912			
4900	10.000	30.510	20.936	46.912			
5000	10.000	30.712	21.130	47.912			
5100	10.000	30.910	21.319	48.912			
5200	10.000	31.104	21.506	49.912			
5300	10.000	31.295	21.689	50 912			
5400	10.000	31.482	21.869	51. 12			
5500	10.000	31.665	22.045	52.912			
5600	10.000	31.845	22.218	53.912			
5700	10.000	32.022	22.388	54.912			
5800	10.000	32.196	22.556	55.912			
5891	10.000	32.352	22.706	56.822			
5891	9.687	64.988	22.706	249.087			
5900	9.688	65.003	22.770	249.174			
6000	9.753	65.166	23.475	250.146			

May 1962 CHW

TUNGSTEN (W) (REFERENCE STATE) gfw = 183.86

0 °K to 3650 °K Crystal

3650 °K to 5891 °K Liquid

5891 °K to 6000 °K Ideal Monatomic Gas

$\Delta H^o_{f0} = 0$

$\Delta H^o_{f298.15} = 0$

$\Delta H^o_{s298.15} = 203.100$ Kcal gfw^{-1}

$S^o_{298.15} = 7.830$ cal degK^{-1} gfw^{-1}

$T_m = 3650$ °K

$\Delta H_m = 8.395$ Kcal gfw^{-1}

$T_b = 5891$ °K

$\Delta H_v = 192.265$ Kcal gfw^{-1}

$H^o_{298.15} - H^o_0 = 1.195$ Kcal gfw^{-1}

$C^o_p = 4.70 + 1.5 \times 10^{-3}T$ cal degK^{-1} gfw^{-1} $\quad 130°K \leq T \leq 3650°K$

$C^o_p = 10$ cal degK^{-1} gfw^{-1} $\quad 3650°K \leq T \leq 5891°K$

Structure

Tungsten exists with the b. c. c. structure.

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Low temperature data by Clusius and Franzosini[1] These data were joined smoothly to the equation given above based on Schomaker et al[2]. Data for liquid tungsten were estimated.

Melting

Several values had been reported. The value adopted is consistent with several other computations.

Vaporization

Based on two experimental determinations. See Barriault *et al*[3] for details.

References

1. Clusius, K., and P. Franzosini, Z. Naturforsch. A14 99 (1959).
2. Schomaker, V., *et al*, Contract DA-30-069-ORD-2787, Prog. Rept. (31 Dec. 1960).
3. Barriault, R., *et al*, ASD TR-61-260 May (1962), Pt. I.

TUNGSTEN (W) (REFERENCE STATE) GFW = 183.86

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T (cal/°K gfw)	$-(F^o_T - H^o_{298})/T$ (cal/°K gfw)	$H^o_T - H^o_{298}$ (Kcal/gfw)	ΔH^o_f (Kcal/gfw)	ΔF^o_f (Kcal/gfw)	Log K_p
298.15	± 0.100	± 0.050	± 0.050	± 0.000			
1000	± 0.500	± 0.410	± 0.200	± 0.210			
2000	± 0.500	± 0.760	± 0.410	± 0.710			
3000	± 1.000	± 1.060	± 0.570	± 1.460			
3650	± 1.500	± 1.300	± 0.680	± 2.270			
3650	± 2.000	± 1.580	± 0.680	± 3.270			
4000	± 2.000	± 1.760	± 0.770	± 3.970			
5000	± 3.000	± 2.320	± 1.030	± 6.470			
5891	± 4.000	± 2.890	± 1.260	± 9.590			
5891	± 0.007	± 0.005					
6000	± 0.007	± 0.005					

TABLE 246

TUNGSTEN — IDEAL MONATOMIC GAS — W

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid W from 0° to 3650°K, Liquid W from 3650° to 5891°K, Gaseous W from 5891° to 6000°K.

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.486	202.809	202.809	INFINITE
298.15	5.092	41.551	41.551	0.000	203.100	193.046	-141.500
300	5.097	41.583	41.551	0.009	203.098	192.983	-140.582
400	5.536	43.101	41.755	0.538	203.039	189.631	-103.604
500	6.297	44.413	42.158	1.128	203.028	186.272	-81.415
600	7.251	45.643	42.637	1.804	203.097	182.927	-66.628
700	7.218	46.835	43.152	2.578	203.257	179.541	-56.053
800	9.026	47.987	43.685	3.442	203.499	176.151	-48.120
900	9.577	49.085	44.224	4.375	203.804	172.697	-41.935
1000	9.586	50.111	44.762	5.348	204.145	169.244	-36.986
1100	9.904	51.054	45.292	6.338	204.495	165.714	-32.923
1200	9.788	51.912	45.809	7.324	204.835	162.197	-29.539
1300	9.569	52.687	46.308	8.292	205.144	158.607	-26.663
1400	9.298	53.387	46.789	9.236	205.415	155.015	-24.198
1500	9.008	54.018	47.251	10.151	205.643	151.407	-22.059
1600	8.721	54.590	47.692	11.038	205.827	147.784	-20.185
1700	8.451	55.111	48.113	11.896	205.968	144.153	-18.531
1800	8.206	55.587	48.515	12.729	206.068	140.513	-17.060
1900	7.987	56.025	48.899	13.538	206.130	136.870	-15.743
2000	7.797	56.429	49.266	14.327	206.155	133.220	-14.557
2100	7.635	56.806	49.616	15.098	206.150	129.576	-13.485
2200	7.500	57.158	49.951	15.855	206.114	125.930	-12.509
2300	7.391	57.489	50.271	16.599	206.051	122.286	-11.619
2400	7.306	57.801	50.579	17.334	205.963	118.646	-10.804
2500	7.243	58.098	50.874	18.061	205.853	115.010	-10.054
2600	7.201	58.381	51.157	18.783	205.722	111.379	-9.362
2700	7.179	58.653	51.430	19.502	205.574	107.752	-8.721
2800	7.173	58.913	51.692	20.220	205.409	104.132	-8.127
2900	7.184	59.165	51.946	20.937	205.229	100.520	-7.575
3000	7.209	59.409	52.190	21.657	205.036	96.909	-7.059
3100	7.247	59.646	52.427	22.380	204.832	93.310	-6.578
3200	7.297	59.877	52.656	23.107	204.616	89.718	-6.127
3300	7.357	60.103	52.878	23.839	204.391	86.130	-5.704
3400	7.426	60.323	53.094	24.578	204.157	82.552	-5.306
3500	7.503	60.540	53.304	25.325	203.917	78.974	-4.931
3600	7.586	60.752	53.508	26.079	203.668	75.413	-4.578
3650	7.630	60.857	53.608	26.460	203.543	73.631	-4.409
3650	7.630	60.857	53.608	26.460	195.148	73.631	-4.409
3700	7.675	60.961	53.706	26.842	195.030	71.969	-4.251
3800	7.769	61.167	53.900	27.615	194.803	68.647	-3.948
3900	7.866	61.370	54.089	28.396	194.584	65.325	-3.661
4000	7.965	61.570	54.274	29.118	194.376	62.016	-3.388
4100	8.067	61.768	54.454	29.989	194.177	58.704	-3.129
4200	8.169	61.964	54.630	30.801	193.989	55.401	-2.883
4300	8.273	62.157	54.803	31.623	193.813	52.116	-2.649
4400	8.376	62.349	54.973	32.456	193.644	48.818	-2.425
4500	8.478	62.538	55.139	33.298	193.486	45.522	-2.211
4600	8.580	62.726	55.301	34.151	193.339	42.242	-2.007
4700	8.680	62.911	55.461	35.014	193.202	38.963	-1.812
4800	8.778	63.095	55.619	35.887	193.075	35.674	-1.624
4900	8.874	63.277	55.773	36.770	192.958	32.399	-1.445
5000	8.968	63.457	55.925	37.662	192.850	29.125	-1.273
5100	9.059	63.636	56.074	38.563	192.751	25.352	-1.108
5200	9.148	63.812	56.221	[illegible]	192.661	[illegible]	-0.949
5300	9.234	63.988	56.366	[illegible]	192.581	18.312	-0.755
5400	9.317	64.161	56.509	41.320	192.508	16.043	-0.649
5500	9.397	64.333	56.650	42.256	192.444	12.771	-0.507
5600	9.474	64.503	56.788	43.199	192.387	9.509	-0.371
5700	9.548	64.671	56.925	44.150	192.338	6.242	-0.239
5800	9.619	64.838	57.060	45.109	192.297	2.975	-0.112
5891	9.682	64.988	57.181	45.987	192.265	0.000	0.000
5891	9.682	64.988	57.181	45.987			
5900	9.688	65.003	57.193	46.074			
6000	9.753	65.166	57.325	47.046			

May 1962 — CHW

TUNGSTEN, MONATOMIC (W) (IDEAL GAS) gfw = 183.86

ΔH^o_{f0} = 202.809 Kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 203.100 Kcal gfw^{-1}

Ground State Configuration $^5D_0$

$S^o_{298.15}$ = 41.551 cal $degK^{-1}$ gfw^{-1}

$H^o_{298.15} - H^o_0$ 1.486 Kcal gfw^{-1}

Electronic levels and multiplicities

Atomic energy levels from Moore[1].

Heat of Formation

Based on experimental vaporization studies by Jones *et al*[2] and Zwikker[3]. Details given by Barriault *et al*[4].

Heat Capacity and Entropy

Calculated on monatomic gas computer program.

References

1. Moore, C., Atomic Energy Levels, Vol. III, Nat. Bur. Stds. (1958).
2. Jones, H. A., I. Langmiur, G. MacKay, Phys. Rev. 30, 201 (1927).
3. Zwikker, C., Physica 5, 249 (1925).
4. Barriault, R., *et al*, ASD TR-61-260(May 1962), Pt. I.

TUNGSTEN, MONATOMIC (W) (IDEAL GAS) GFW = 183.86

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	cal/°K gfw			Kcal gfw			
	C^o_p	S^o_T	$-(F^o_T - H^o_{298})/T$	$H^o_T - H^o_{298}$	ΔH^o_f	ΔF^o_f	Log K_p
298.15	± 0.000	± 0.002	± 0.002	± 0.000	± 1.800	± 1.820	± 1.330
1000	± 0.001	± 0.003	± 0.003	± 0.001	± 2.010	± 2.000	± 0.440
2000	± 0.001	± 0.003	± 0.003	± 0.001	± 2.510	± 2.630	± 0.290
3000	± 0.001	± 0.003	± 0.003	± 0.002	± 3.260	± 3.520	± 0.260
3650	± 0.002	± 0.003	± 0.003	± 0.002	± 4.070	± 4.290	± 0.260
3650	± 0.002	± 0.003	± 0.003	± 0.002	± 5.070	± 4.290	± 0.260
4000	± 0.003	± 0.003	± 0.003	± 0.003	± 5.770	± 4.890	± 0.270
5000	± 0.006	± 0.004	± 0.003	± 0.007	± 8.280	± 6.970	± 0.300
5891	± 0.007	± 0.005	± 0.003	± 0.012	± 1.140	± 9.240	± 0.340
5891	± 0.007	± 0.005	± 0.003	± 0.012			
6000	± 0.007	± 0.005	± 0.003	± 0.013			

TABLE 247

YTTRIUM — REFERENCE STATE — Y

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Y from 0° to 1803°K, Liquid Y from 1803° to 3605°K, Gaseous Y from 3605° to 6000°K.

T, °K	cal/°K gfw C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	Kcal/gfw $H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.426			
298.15	6.349	10.630	10.630	0.000			
300	6.352	10.669	10.630	0.012			
400	6.509	12.518	10.881	0.655			
500	6.669	13.987	11.360	1.314			
600	6.832	15.218	11.903	1.989			
700	6.998	16.283	12.455	2.680			
800	7.168	17.229	12.993	3.388			
900	7.340	18.083	13.512	4.114			
1000	7.516	18.865	14.009	4.857			
1100	7.695	19.590	14.484	5.617			
1200	7.876	20.267	14.938	6.396			
1300	8.061	20.905	15.373	7.192			
1400	8.249	21.509	15.789	8.008			
1500	8.441	22.085	16.190	8.842			
1600	8.635	22.636	16.576	9.696			
1700	8.832	23.165	16.948	10.569			
1758	8.948	23.464	17.158	11.085			
1758	8.371	24.140	17.158	12.274			
1800	8.371	24.338	17.323	12.626			
1803	8.371	24.352	17.335	12.651			
1803	10.303	25.867	17.335	15.383			
1900	10.303	26.407	17.784	16.382			
2000	10.303	26.935	18.229	17.412			
2100	10.303	27.438	18.656	18.443			
2200	10.303	27.917	19.066	19.473			
2300	10.303	28.375	19.461	20.503			
2400	10.303	28.814	19.841	21.534			
2500	10.303	29.234	20.209	22.564			
2600	10.303	29.638	20.564	23.594			
2700	10.303	30.027	20.907	24.625			
2800	10.303	30.402	21.239	25.655			
2900	10.303	30.763	21.562	26.685			
3000	10.303	31.113	21.874	27.715			
3100	10.303	31.450	22.178	28.746			
3200	10.303	31.778	22.473	29.776			
3300	10.303	32.095	22.759	30.806			
3400	10.303	32.402	23.038	31.837			
3500	10.303	32.701	23.310	32.867			
3600	10.303	32.991	23.575	33.897			
3604.68	10.303	33.004	23.587	33.945			
3604.68	8.004	57.262	23.587	120.623			
3700	8.237	57.485	24.452	121.396			
3800	8.477	57.708	25.318	122.232			
3900	8.714	57.931	26.146	123.092			
4000	8.944	58.155	26.937	123.975			
4100	9.166	58.378	27.696	124.880			
4200	9.380	58.602	28.424	125.808			
4300	9.583	58.824	29.124	126.756			
4400	9.774	59.046	29.796	127.724			
4500	9.954	59.266	30.443	128.710			
4600	10.121	59.486	31.068	129.714			
4700	10.276	59.704	31.670	130.734			
4800	10.417	59.920	32.251	1[illegible]769			
4900	10.544	60.134	32.814	132.817			
5000	10.659	60.346	33.359	133.877			
5100	10.761	60.556	33.885	134.948			
5200	10.850	60.763	34.396	136.029			
5300	10.927	60.968	34.892	137.118			
5400	10.992	61.170	35.373	138.214			
5500	11.046	61.370	35.840	139.316			
5600	11.090	61.566	36.294	140.423			
5700	11.123	61.760	36.735	141.529			
5800	11.148	61.951	37.166	142.647			
5900	11.164	62.138	37.584	143.763			
6000	11.172	62.327	37.992	144.880			

15 Marcy 1963 — MG

$0^{o}K$ to $1803^{o}K$	Crystal
$1803^{o}K$ to $3605^{o}K$	Liquid
$3605^{o}K$ to $6000^{o}K$	Ideal Monatomic Gas

$\Delta H^{o}_{f0} = 0$

$\Delta H^{o}_{f298.15} = 0$

$\Delta H^{o}_{s298.15} = 101.326$ Kcal gfw^{-1}

$S^{o}_{298.15} = 10.630$ cal degK^{-1} gfw^{-1}

$T_t = 1758^{o}K$

$\Delta H_t = 1.189$ Kcal gfw^{-1}

$T_m = 1803^{o}K$

$\Delta H_m = 2.732$ Kcal gfw^{-1}

$T_b = 3604.68^{o}K$

$\Delta H_v = 86.678$ Kcal gfw^{-1}

$H^{o}_{298.15} - H^{o}_{0} = 1.426$ Kcal gfw^{-1}

$C^{o}_{p} = 5.899 + 1.462 \times 10^{-3}T + 15.492 \times 10^{-8}T^{2}$ cal degK^{-1} gfw^{-1}

$$273.15^{o}K \leq T \leq 1758^{o}K$$

$C^{o}_{p} = 8.371$ cal degK^{-1} gfw^{-1} for $1758^{o} \leq T \leq 1803^{o}K$; $C^{o}_{p} = 10.303$ cal degK^{-1}gfw^{-1} for liquid

Structure.

h. c. p. to $1758^{o}K$; b. c. c. from 1758^{o} to $1803^{o}K$

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Low temperature data by Jennings *et al.*[1] High temperature data by Berg.[2]

Melting

Melting points, heat of transition, and heat of fusion from Berg.[2]

Heat of Sublimation

Vaporization data from Ackermann and Rauh[3] were used.

References

1. Jennings, L. D., R. E. Miller and F. H. Spedding, J. Chem. Phys. 33, 1849 (1960)
2. Berg, J. R., Ph.D. Thesis, Iowa State Univ. (1961).
3. Ackermann, R J. and E. G. Rauh, J. Chem. Phys. 36, 448 (1962).

TABLE 248

YTTRIUM — IDEAL MONATOMIC GAS — Y

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Y from 0° to 1803°K, Liquid Y from 1803° to 3605°K, Gaseous Y from 3605° to 6000°K

T, °K	cal/°K gfw			Kcal/gfw			
	C_p°	S_T°	$-(F_T^\circ - H_{298}^\circ)/T$	$H_T^\circ - H_{298}^\circ$	ΔH_f°	ΔF_f°	Log K_p
0	0.000	0.000	INFINITE	-1.639	101.539	101.539	INFINITE
298.15	6.181	42.870	42.870	0.000	101.326	91.714	-67.225
300	6.181	42.909	42.871	0.011	101.325	91.654	-66.767
400	6.045	44.673	43.112	0.624	101.295	88.434	-48.316
500	5.826	45.999	43.563	1.218	101.230	85.225	-37.250
600	5.638	47.044	44.059	1.791	101.128	82.033	-29.879
700	5.494	47.901	44.548	2.347	100.993	78.861	-24.620
800	5.388	48.628	45.014	2.891	100.829	75.709	-20.682
900	5.308	49.258	45.451	3.426	100.638	72.581	-17.624
1000	5.249	49.814	45.860	3.953	100.422	69.475	-15.183
1100	5.203	50.312	46.243	4.476	100.185	66.391	-13.190
1200	5.169	50.763	46.601	4.994	99.924	63.331	-11.534
1300	5.144	51.175	46.937	5.510	99.644	60.293	-10.136
1400	5.127	51.556	47.254	6.023	99.341	57.275	-8.941
1500	5.119	51.909	47.552	6.536	99.020	54.283	-7.909
1600	5.120	52.240	47.835	7.047	98.677	51.312	-7.009
1700	5.130	52.550	48.103	7.560	98.317	48.363	-6.217
1758	5.143	52.721	48.251	7.590	97.831	46.665	-5.801
1758	5.143	52.721	48.251	7.590	96.642	46.665	-5.801
1800	5.153	52.844	48.359	8.074	96.774	45.461	-5.520
1803	5.154	52.852	48.366	8.090	96.765	45.377	-5.500
1803	5.154	52.852	48.366	8.090	94.033	45.377	-5.500
1900	5.187	53.124	48.602	8.591	93.535	42.772	-4.920
2000	5.235	53.391	48.835	9.112	93.026	40.114	-4.383
2100	5.298	53.648	49.058	9.638	92.521	37.482	-3.901
2200	5.377	53.896	49.272	10.172	92.025	34.873	-3.464
2300	5.472	54.137	49.479	10.714	91.537	32.285	-3.068
2400	5.584	54.372	49.678	11.267	91.059	29.718	-2.706
2500	5.713	54.603	49.870	11.832	90.594	27.174	-2.375
2600	5.858	54.830	50.056	12.410	90.142	24.647	-2.072
2700	6.020	55.054	50.237	13.004	89.705	22.135	-1.792
2800	6.198	55.276	50.413	13.615	89.286	19.639	-1.533
2900	6.389	55.497	50.585	14.244	88.885	17.160	-1.293
3000	6.594	55.717	50.752	14.893	88.504	14.692	-1.070
3100	6.810	55.936	50.916	15.563	88.143	12.238	-0.863
3200	7.035	56.156	51.076	16.255	87.805	9.797	-0.669
3300	7.268	56.376	51.234	16.970	87.490	7.359	-0.487
3400	7.507	56.597	51.388	17.709	87.198	4.936	-0.317
3500	7.750	56.818	51.540	18.472	86.931	2.521	-0.157
3600	7.993	57.039	51.690	19.259	86.688	0.112	-0.007
3604.68	8.004	57.049	51.697	19.297	86.678	-0.001	0.000
3604.68	8.004	57.049	51.697	19.297			
3700	8.237	57.262	51.837	20.070			
3800	8.477	57.485	51.983	20.906			
3900	8.714	57.708	52.127	21.766			
4000	8.944	57.931	52.269	22.649			
4100	9.166	58.155	52.410	23.554			
4200	9.380	58.378	52.549	24.482			
4300	9.583	58.602	52.688	25.430			
4400	9.774	58.824	52.825	26.398			
4500	9.954	59.046	52.960	27.384			
4600	10.121	59.266	53.095	28.388			
4700	10.276	59.486	53.229	29.408			
4800	10.417	59.704	53.361	30.443			
4900	10.544	59.920	53.493	31[illegible]91			
5000	10.659	60.134	53.624	32.[illegible]1			
5100	10.761	60.346	53.753	33.622			
5200	10.850	60.556	53.882	34.703			
5300	10.927	60.763	54.010	35.792			
5400	10.992	60.968	54.137	36.888			
5500	11.046	61.170	54.263	37.990			
5600	11.090	61.370	54.388	39.097			
5700	11.123	61.566	54.512	40.208			
5800	11.148	61.760	54.636	41.321			
5900	11.164	61.951	54.758	42.437			
6000	11.172	62.138	54.880	43.554			

15 March 1963 — MG

ΔH^o_{f0} = 101.539 Kcal gfw^{-1}

Ground State Configuration $^2D_{3/2}$

$H^o_{298.15}-H^o_0$ = 1 639 Kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 101.326 Kcal gfw^{-1}

$S^o_{298.15}$ = 42.870 cal degK^{-1} gfw^{-1}

Electronic Levels and Multiplicities

Energy levels from Moore.[1]

Heat of Formation

Based on data of Ackermann and Rauh.[2]

Heat Capacity and Entropy

Calculated on monatomic gas program.

References

1. Moore, C. E., Nat. Bur. Std. (U.S.), Circ. 467, Vol. II (1952).
2. Ackermann, R. J. and E. G. Rauh, J. Chem. Phys. 36, 448 (1962).

TABLE 249

ZIRCONIUM **REFERENCE STATE** **Zr**

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Zr from 0° to 2125°K, Liquid Zr from 2125° to 4644°K, Gaseous Zr from 4644° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.313			
298.15	6.001	9.290	9.290	0.000			
300	6.015	9.327	9.290	0.011			
400	6.555	11.140	9.534	0.642			
500	6.882	12.640	10.009	1.315			
600	7.124	13.917	10.557	2.016			
700	7.327	15.031	11.118	2.739			
800	7.508	16.021	11.670	3.481			
900	7.677	16.915	12.204	4.240			
1000	7.838	17.732	12.717	5.016			
1100	7.994	18.487	13.207	5.808			
1135	8.048	18.738	13.374	6.088			
1135	7.900	19.544	13.374	7.003			
1200	7.900	19.984	13.720	7.517			
1300	7.900	20.617	14.227	8.307			
1400	7.900	21.202	14.704	9.097			
1500	7.900	21.747	15.156	9.887			
1600	7.900	22.257	15.584	10.677			
1700	7.900	22.736	15.991	11.467			
1800	7.900	23.187	16.378	12.257			
1900	7.900	23.614	16.748	13.047			
2000	7.900	24.020	17.101	13.837			
2100	7.900	24.405	17.440	14.627			
2125	7.900	24.499	17.523	14.824			
2125	8.000	26.805	17.523	19.724			
2200	8.000	27.087	17.844	20.324			
2300	8.000	27.438	18.253	21.124			
2400	8.000	27.778	18.643	21.924			
2500	8.000	28.105	19.015	22.724			
2600	8.000	28.418	19.371	2[illegible].524			
2700	8.000	28.720	19.711	24.324			
2800	8.000	29.011	20.038	25.124			
2900	8.000	29.292	20.353	25.924			
3000	8.000	29.563	20.655	26.724			
3100	8.000	29.826	20.947	27.524			
3200	8.000	30.080	21.228	28.324			
3300	8.000	30.326	21.500	29.124			
3400	8.000	30.565	21.763	[illegible].[illegible]24			
3500	8.000	30.796	22.018	30.724			
3600	8.000	31.022	22.265	31.524			
3700	8.000	31.241	22.505	32.324			
3800	8.000	31.454	22.737	33.124			
3900	8.000	31.662	22.964	33.924			
4000	8.000	31.865	23.184	34.72[illegible]			
4100	8.000	32.062	23.398	35.524			
4200	8.000	32.255	23.606	36.324			
4300	8.000	32.443	23.810	37.124			
4400	8.000	32.627	24.008	37.924			
4500	8.000	32.807	24.202	38.724			
4600	8.000	32.983	24.391	39.524			
4644.05	8.000	33.059	24.473	39.876			
4644.05	8.952	62.226	24.473	175.330			
4700	8.984	62.334	24.923	175.832			
4800	9.039	62.524	25.704	176.733			
4900	9.091	62.711	26.458	1[illegible]640			
5000	9.139	62.895	27.185	178.551			
5100	9.185	63.076	27.886	179.467			
5200	9.226	63.255	28.565	180.388			
5300	9.265	63.431	29.221	181.313			
5400	9.300	63.605	29.856	182.241			
5500	9.332	63.775	30.471	183.172			
5600	9.361	63.944	31.068	184.107			
5700	9.387	64.110	31.646	185.045			
5800	9.409	64.273	32.207	185.984			
5900	9.429	64.434	32.752	186.926			
6000	9.446	64.593	33.282	187.870			

15 March 1963 HLS

0°K to 2125°K	Crystal
2125°K to 4644.05°K	Liquid
4644.05°K to 6000°K	Ideal Monatomic Gas

$\Delta H^o_{f0} = 0$

$\Delta H^o_{f298.15} = 0$

$\Delta H^o_{s298.15} = 143.126$ Kcal gfw^{-1}

$S^o_{298.15} = 9.29$ cal degK^{-1} gfw^{-1}

$T_t = 1135°K$

$\Delta H_t = 0.915$ Kcal gfw^{-1}

$T_m = 2125°K$

$\Delta H_m = 4.900$ Kcal gfw^{-1}

$T_b = 4644.05°K$

$\Delta H_v = 135.454$ Kcal gfw^{-1}

$H^o_{298.15} - H^o_0 = 1.313$ Kcal gfw^{-1}

$C^o_p = 6.50 + 1.42 \times 10^{-3}T - 0.82 \times 10^5 T^{-2}$ cal degK^{-1}gfw^{-1} $298.15°K \leq T \leq 1135°K$

$C^o_p = 7.900$ cal degK^{-1}gfw^{-1} $1135 \leq T \leq 2125°K$

$C^o_p = 8.00$ cal deg K^{-1} gfw^{-1} $2125 \leq T \leq 4644°K$

Structure

h. c. p. to 1135°K, b. c. c. from 1135°K to melting point

Heat of Formation

Zero by definition.

Heat Capacity and Entropy

Low temperature data from Skinner and Johnston [1] High temperature data from Kelley [2]

Melting

Temperature of transition point and heat of transition from Kelley [2] Heat of fusion from Kelley.[2] Melting temperature from Hultgren *et al* [3]

Heat of Sublimation

An average of the data by Trulson and Goldstein[4] and Skinner *et al* [5]

References

1. Skinner, G B and H L Johnston, J Am. Chem. Soc. 73, 4549 (1951)
2. Kelley, K K, Bur Mines, Bull. 584 (1960)
3. Hultgren, R *et al*, *Selected Values*, U of California, Berkeley (1960)
4. Trulson, O C and H W Goldstein, Union Carbide Quarterly Progress Rept., Contract DA-30-069-2787 (31 March 1962).
5. Skinner, G B, J W Edwards and H L Johnston, J Am. Chem Soc 73, 174 (1951)

ZIRCONIUM (Zr) (REFERENCE STATE) GFW = 91.22

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T (cal/°K gfw)	$-(F^o_T - H^o_{298})/T$ (cal/°K gfw)	$H^o_T - H^o_{298}$ (Kcal/gfw)	ΔH^o_f (Kcal/gfw)	ΔF^o_f (Kcal/gfw)	Log K_p
298.15	± 0.050	± 0.040	± 0.040	± 0.000			
1000	± 0.500	± 0.123	± 0.065	± 0.058			
1135	± 0.500	± 0.185	± 0.077	± 0.123			
1135	± 0.500	± 0.273	± 0.077	± 0.223			
2000	± 1.000	± 0.569	± 0.229	± 0.680			
2125	± 1.000	± 0.625	± 0.251	± 0.796			
2125	± 2.000	± 0.860	± 0.251	± 1.296			
3000	± 2.000	± 1.550	± 0.535	± 3.046			
4000	± 2.000	± 2.125	± 0.864	± 5.046			
4644.05	± 2.000	± 2.465	± 1.088	± 6.532			
4644.05	± 0.002	± 0.004					
5000	± 0.002	± 0.004					
6000	± 0.001	± 0.004					

TABLE 250

ZIRCONIUM IDEAL MONATOMIC GAS Zr

Reference State for Calculating ΔH_f°, ΔF_f°, and Log K_p: Solid Zr from 0° to 2125°K, Liquid Zr from 2125° to 4644°K, Gaseous Zr from 4644° to 6000°K.

T, °K	C_p° (cal/°K gfw)	S_T° (cal/°K gfw)	$-(F_T^\circ - H_{298}^\circ)/T$ (cal/°K gfw)	$H_T^\circ - H_{298}^\circ$ (Kcal/gfw)	ΔH_f° (Kcal/gfw)	ΔF_f° (Kcal/gfw)	Log K_p
0	0.000	0.000	INFINITE	-1.629	142.810	142.810	INFINITE
298.15	6.368	43.317	43.317	0.000	143.126	132.981	-97.473
300	6.375	43.356	43.317	0.012	143.127	132.918	-96.826
400	6.612	45.231	43.571	0.664	143.148	129.511	-70.758
500	6.594	46.707	44.056	1.326	143.137	126.102	-55.117
600	6.464	47.899	44.601	1.979	143.089	122.700	-44.691
700	6.316	48.884	45.144	2.618	143.005	119.308	-37.248
800	6.199	49.719	45.665	3.243	142.888	115.930	-31.669
900	6.133	50.445	46.157	3.859	142.745	112.568	-27.334
1000	6.121	51.090	46.619	4.472	142.582	109.224	-23.870
1100	6.156	51.675	47.052	5.085	142.403	105.897	-21.039
1135	6.177	51.868	47.198	5.301	142.339	104.736	-20.166
1135	6.177	51.868	47.198	5.301	141.424	104.736	-20.166
1200	6.226	52.213	47.460	5.704	141.313	102.638	-18.692
1300	6.320	52.715	47.845	6.331	141.150	99.423	-16.714
1400	6.428	53.188	48.210	6.969	140.998	96.218	-15.020
1500	6.542	53.635	48.557	7.617	140.856	93.024	-13.553
1600	6.655	54.061	48.888	8.277	140.7[illegible]5	89.840	-12.271
1700	6.764	54.468	49.204	8.948	140.607	86.664	-11.141
1800	6.866	54.857	49.507	9.629	140.498	83.494	-10.137
1900	6.960	55.231	49.799	10.321	140.400	80.329	-9.240
2000	7.047	55.590	50.080	11.021	140.310	77.168	-8.432
2100	7.128	55.936	50.350	11.730	140.229	74.015	-7.702
2125	7.148	56.020	50.416	11.909	140.211	73.228	-7.531
2125	7.148	56.020	50.416	11.909	135.311	73.228	-7.531
2200	7.204	56.269	50.612	12.447	135.249	71.036	-7.056
2300	7.276	56.591	50.865	13.171	135.173	68.118	-6.472
2400	7.345	56.902	51.110	13.902	135.104	65.205	-5.937
2500	7.413	57.204	51.348	14.640	135.042	62.294	-5.445
2600	7.481	57.496	51.578	15.384	134.986	59.388	-4.992
2700	7.549	57.779	51.803	16.136	134.938	56.478	-4.571
2800	7.618	58.055	52.021	16.894	134.896	53.574	-4.181
2900	7.688	58.323	52.234	17.659	134.861	50.671	-3.818
3000	7.760	58.585	52.441	18.432	134.834	47.768	-3.480
3100	7.833	58.841	52.644	19.212	134.814	44.865	-3.163
3200	7.908	59.091	52.841	19.999	134.801	41.964	-2.866
3300	7.984	59.335	53.034	20.793	134.79[illegible]	39.064	-2.587
3400	8.061	59.575	53.223	21.595	134.797	36.162	-2.324
3500	8.139	59.810	53.408	22.405	134.807	33.261	-2.077
3600	8.217	60.040	53.589	23.223	134.825	30.360	-1.843
3700	8.294	60.266	53.767	24.049	134.8[illegible]	27.457	-1.622
3800	8.371	60.488	53.941	24.882	134.884	24.551	-1.412
3900	8.447	60.707	54.111	25.723	134.925	21.653	-1.213
4000	8.522	60.922	54.279	26.571	134.973	18.746	-1.024
4100	8.595	61.133	54.443	27.427	135.029	15.842	-0.844
4200	8.666	61.341	54.605	28.290	135.092	12.930	-0.673
4300	8.735	61.546	54.764	29.160	135.162	10.024	-0.509
4400	8.802	61.747	54.921	30.037	135.239	7.109	-0.353
4500	8.865	61.946	55.075	30.921	135.323	4.198	-0.204
4600	8.926	62.141	55.226	31.810	135.412	1.285	-0.061
4644.05	8.952	62.226	55.292	32.204	135.454	0.001	0.000
4644.05	8.952	62.226	55.292	32.204			
4700	8.984	62.334	55.375	32.706			
4800	9.039	62.524	55.522	3[illegible].07			
4900	9.091	62.711	55.667	34.[illegible]14			
5000	9.139	62.895	55.810	35.425			
5100	9.185	63.076	55.950	36.341			
5200	9.226	63.255	56.089	37.262			
5300	9.265	63.431	56.226	38.187			
5400	9.300	63.605	56.361	39.115			
5500	9.332	63.775	56.494	40.046			
5600	9.361	63.944	56.626	40.981			
5700	9.387	64.110	56.756	41.919			
5800	9.409	64.273	56.884	42.858			
5900	9.429	64.434	57.011	43.800			
6000	9.446	64.593	57.136	44.744			

15 March 1963 HLS

ZIRCONIUM, MONATOMIC (Zr) (IDEAL GAS) gfw = 91.22

ΔH^o_{f0} = 142.810 Kcal gfw^{-1}

Ground State Configuration $^3F_2$

$H^o_{298.15}-H^o_0$ = 1.629 Kcal gfw^{-1}

$\Delta H^o_{f298.15}$ = 143.126 Kcal gfw^{-1}

$S^o_{298.15}$ = 43.317 cal degK^{-1}gfw^{-1}

Electronic Levels and Multiplicities

All levels from Moore.[1]

Heat of Formation

An average heat of formation based on the work of Trulson and Goldstein[2] and Skinner *et al*[3] was used.

Heat Capacity and Entropy

Calculated using monatomic gas program.

References

1. Moor , C., Atomic Energy Levels, Vol. 2 (1952).
2. Trulson, O. C. and H. W. Goldstein, in Union Carbide Quarterly Progress Rept. by Lowrie *et al* under Contract DA-30-069-2787 (31 March 1962).
3. Skinner, G. B., J. W. Edwards and H. L. Johnston, J. Am. Chem. Soc. 73, 174 (1951).

ZIRCONIUM, MONATOMIC (Zr) (IDEAL GAS) GFW = 91.22

SUMMARY OF UNCERTAINTY ESTIMATES

T, °K	C^o_p (cal/°K gfw)	S^o_T (cal/°K gfw)	$-(F^o_T - H^o_{298})/T$ (cal/°K gfw)	$H^o_T - H^o_{298}$ (Kcal/gfw)	ΔH^o_f (Kcal/gfw)	ΔF^o_f (Kcal/gfw)	Log K_p
298.15	± 0.001	± 0.002	± 0.003	± 0.000	± 4.000		
1000	± 0.001	± 0.002	± 0.003	± 0.000			
1135	± 0.001	± 0.002	± 0.003	± 0.000			
1135	± 0.001	± 0.002	± 0.003	± 0.000			
2000	± 0.001	± 0.003	± 0.003	± 0.001			
2125	± 0.001	± 0.003	± 0.003	± 0.001			
2125	± 0.001	± 0.003	± 0.003	± 0.001			
3000	± 0.002	± 0.003	± 0.003	± 0.002			
4000	± 0.002	± 0.003	± 0.003	± 0.003			
4644.05	± 0.002	± 0.004	± 0.003	± 0.005			
5000	± 0.002	± 0.004	± 0.003	± 0.005			
6000	± 0.001	± 0.004	± 0.003	± 0.006			

VIII
BIBLIOGRAPHY

BIBLIOGRAPHY
AND
PROPERTY FILE

This document, volume 2, provides a key to much thermodynamic and related literature for refractories of interest. A bibliography (section VIII) and subject or property file (section IX) are included herein. The present bibliography has been utilized in the work reported in volume 1 (Discussion) and volume 2 (Thermodynamic Tables).

Basically, the present bibliography has been compiled by finding pertinent references for 35 elements, and their borides, carbides, nitrides, and oxides. The elements of interest include: beryllium, boron, calcium, carbon, cerium, chromium, dysprosium, gadolinium, hafnium, iridium, lanthanum, magnesium, manganese, molybdenum, niobium, nitrogen, neodymium, osmium, oxygen, platinum, rhenium, rhodium, samarium, scandium, silicon, strontium, tantalum, technetium, thorium, titanium, tungsten, uranium, vanadium, yttrium, and zirconium.

The manner of compiling this bibliography has been described in section IIB of volume 1. For complete information, that section should be consulted. Many abstracting sources have been utilized. The literature available through October 1963 Chemical Abstracts has been included herein.

The authors are well aware of many deficiencies of the present work, and no claim is made for completeness. An earlier bibliography[1] can be consulted for further references. There may be a small amount of duplication of that earlier work by this work, but in general this is not expected to be too large. The references cited in this bibliography may often contain data of a nonthermodynamic nature. However, if it appeared that the article might provide useful complementary material, it was included. Also, in some cases, data for compounds of not immediate interest have been included because of their relationships to compounds which are of interest.

It is felt that the present bibliography can provide a good basis for the investigation of thermodynamic properties of the given compounds. However, the careful worker who wants a very complete bibliography must expect to delve deeper by further cross referencing, by usage of abstract indexes, etc. For example, in the analyses of volume 1, many references have been discovered which are not in the bibliography.

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[1] Barriault, R. J. et al, ASD TR 61-260, Pt. I, Vol. 2 (May 1962).

Manuscript released by authors (December 1963) for publication as an ASD Technical Documentary Report.

In utilizing the present bibliography, one normally should consult the subject or property file (section IX) first. A given compound is listed in column ②, of this file, by the usual chemical formula arranged alphabetically. Once, a particular compound has been found, desired properties can be selected from column ①. In this column, a mnemonic code has been used. For codes which are not immediately obvious, one can consult the property-file-code sheet at the beginning of section IX. After a desired reference is located in the property or subject file of section IX, it can then be located in the alphabetic or main bibliography of section VIII. To locate it there, one uses the information in the last three columns (③, ④, ⑤) of the property file of section IX. Usually, the author's name will be sufficient, but the year information and the code number in the last column provide the positive identification of a particular reference.

Column ① - identifies the left-most column in heavy print on the first, alternate lines for a given reference. It refers to SPK, THER, THER, TRT, etc., on the sample page of the property file.

Column ② - identifies the second or right-most column, in light print on the first, alternate lines for a given reference. It refers to TC, TC, etc., on the sample page of the property file.

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CA 55, 19698 (1961) 300549
NS 15, 17343 (1961) 300549

ZHURAVLEV, N STEPANØVA, A 700727
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IX
PROPERTY FILE

PROPERTY FILE CODE

ACT	ACTIVITY
BETA	COMPRESSIBILITY COEFFICIENT (BETA = 1/V*(DV/DP) T
BIB	BIBLIOGRAPHY
BOOK	BOOK
CEMP	CONDENSED PHASE, ELEC OR MAGNETIC PROP, EG WORK FUNC
COPT	CONDENSED PHASE, OPTICAL PROP.
CPH	HIGH TEMPERATURE HEAT CAPACITY
CPL	LOW TEMPERATURE HEAT CAPACITY
CRYS	CRYSTAL STRUCTURE
CTEX	COEFF OF THERMAL EXPANSION
DF	FREE ENERGY OF FORMATION, REACTION, ETC.
DH	HEAT OF FORMATION, REACTION, ETC
DHD	DISSOCIATION ENERGY
DHT	HEAT OF TRANSFORMATION
E	INTERNAL ENERGY
ELCH	ELECTROCHEMICAL
EMF	ELECTROMOTIVE FORCE
ENG	ENERGY LEVELS
ERES	ELECTRICAL RESISTIVITY
EXAPP	EXPERIMENTAL APPARATUS
EXPRO	EXPERIMENTAL PROBLEM
EXPTL	EXPERIMENTAL
EXTEC	EXPERIMENTAL TECHNIQUE
F	FREE ENERGY FUNCTION
H	HEAT CONTENT
KIN	KINETICS
MISC	MISCELLANEOUS
MPP	MISCELLANEOUS PHYSICAL PROPERTIES
MSP	MASS SPECTROMETRIC DATA
PHAS	PHASE DATA, MELTING, TRANSITION, BOILING TEMPS
PMCH	MECHANICAL PROPERTIES
PREP	PREPARATION OF MATERIAL
REAC	CHEMICAL REACTIONS
REV	REVIEW
RHO	DENSITY
S	ENTROPY
SPK	SPECTROSCOPIC DATA
SURF	SURFACE PROPERTIES
TCON	THERMAL CONDUCTIVITY
THEO	THEORY
THER	THERMODYNAMIC DATA
TRT	TRANSFORMATION TEMPERATURES
VAP	VAPORIZATION DATA
ZKP	EQ CONST

CRYS	B	KOLAKOWSKI	62	301508
CRYS	B	CARPENTER, R KATO,	60	600826
CRYS	B	KOHN, J NYE, W GA	60	600881
DH	B	ROBSON, H	58	300275
DH	B	AKISHIN, P NIKITIN	59	300352
ERES	B	HOOD, C THURSTON,	62	601694
ERES	B	SAMSONOV, G	61	700587
ERES	B	TAYLOR, W ET AL	61	301602
KIN	B	SLEPTSOV, V SAMSON	60	200768
MISC	B	SAMSONOV, G	60	200916
MSP	B	SHAPIRO, I WILSON,	61	201356
PHAS	B	HOOD, C THURSTON,	62	601694
PHAS	B	MARTIN, R SEAGLE,	61	300308
PHAS	B	DOLLOFF, R	60	700989
PHAS	B	BECHER, H	61	300343
PHAS	B	TALLEY, C POST, B	60	200993
REAC	B	ELLIS, R	60	200980
REAC	B	ROSENBERY, J	60	201392
REAC	B	GILLES, P	61	201334
REAC	B	VEKSHINA, N MARKOV	62	201487
PHAS	B	KOHN, J NYE, W GA	60	600881
REAC	B	FISHER, F	60	200877
REAC	B	FEDEROV, T F SHAMA	60	300197
REAC	B	SAMSONOV, G MARKOV	60	300575
REAC	B	RUSIN, A TATEVSKII	61	301117
REAC	B	HENDERSON, U	62	301469
REV	B	WOHLL, M	60	701053
REV	B	KOHN, J NYE, W GA	60	600881
REV	B	WILLIAMS, D	60	201304
SPK	B	KRAEV, M	61	300798
SPK	B	PILCHER, G SKINNER	62	301044
SPK	B	RUSIN, A TATEVSKII	61	300580
SPK	B	MALTSEV, A KATAEV,	60	600701
SPK	B	KRAEV, M	61	301068
THER	B	SCHICK, H ANTHROP	63	300994
THER	B	SULLIVAN, R SEIBEL	60	701038
THER	B	SAMSONOV, G MARKOV	60	301118
THER	B	WILLIAMS, N N	61	700659
TRT	B	MARTIN, R SEAGLE.	61	300308
TRT	B	DOLLOFF, R	60	600662
VAP	B	KATHAYATE, Y RIHAN	63	301493
VAP	B	PAULE, R	61	601479
VAP	B	PRISELKOV, YU A SA	60	300142
VAP	B	MARGRAVE, J	61	700967
VAP	B	KIBLER, G LYON, T	62	300427
VAP	B	PAULE, R MARGRAVE	63	301320
VAP	B	PRISELKOV, Y SAPOZ	60	600637
PHAS	B SYST	STEPANOVA, A UMANS	56	601204
SPK	B SYST	STEPANOVA, A UMANS	56	601204
PHAS	B AL SYST	SEREBRYANSKII, V	61	300840
CRYS	B C	KUDRYAVTSEVA, V SO	60	600789
PHAS	B C	MARTIN, R SEAGLE,	61	300308
REAC	B C	LENZI, D PELLEGRIN	59	200865
REAC	B C	NAZARCHUK, T	61	201578
TRT	B C	MARTIN, R SEAGLE,	61	300308
CEMP	B 4C	SAMSONOV, G SYNELN	61	300386
REAC	B 4C	BOSCH, F	62	202008
MPP	B 4C	PORTNOY, K SAMSONO	61	300486
REAC	B 4C	LYUTAYA, M NAZARCH	61	300526
CRYS	B 4C	EPELBAUM, V A SEVA	61	300202
REAC	B 4C	VUILLARD, G LUQUE	61	201467
PHAS	B 4C SYST	DOLLOFF, R	60	700969
CRYS	B C SYST	ELLIOTT, R VAN THY	60	701069
ERES	B C SYST	SAMSONOV, G	61	601585
MPP	B C SYST	KISLEY, P S SAMSON	60	300137
MPP	B C SYST	ZHURAVLEV, N MAKAR	61	300549
MSP	B C SYST	VERHAEGEN, G STAFF	62	601660
PHAS	B C SYST	SAMSONOV, G	61	601585
PHAS	B C SYST	ELLIOTT, R VANTHYN	60	600622
PHAS	B C SYST	ELLIOTT, R	61	700718
PHAS	B C SYST	DOLLOFF, R	60	700989
PHAS	B C SYST	ZHURAVLEV, N MAKAR	61	300549
PHAS	B C SYST	DOLLOFF, R	60	600662
THER	B C SYST	SAMSONOV, G	59	201343
REV	B C SYST	ELLIOTT, R THYNE	60	600673
VAP	B C SYST	VERHAEGEN, G STAFF	62	301609
THER	B C SYST	VERHAEGEN, G STAFF	62	601660
THER	B C SYST	VERHAEGEN, G STAFF	60	601574

VAP	B C SYST		
	VERHAEGEN, G STAFF	60	601574
DH	B F 3		
	GALCHENKO, G TIMOF	60	201644
REAC	B 2F 4		
	HOLLIDAY, A TAYLOR	62	201724
CPH	B N		
	WALKER, B EWING, C	62	301098
CPH	B N		
	PROPHET, H STULL	63	300961
CPH	B N		
	MCDONALD, R STULL,	61	300333
DH	B N		
	GALCHENKO, G KORMI	60	201645
KIN	B N		
	SAMSONOV, G SLEPTS	60	201815
CPH	B N		
	MAGNUS, A DANZ, H	26	700580
CRYS	B N		
	THOMAS, J WESTON	62	301039
CRYS	B N		
	WENTORF, R	61	700935
DH	B N		
	WISE, S	62	300741
DH	B N		
	HILDENBRAND, D L	61	300219
H	B N		
	MEZAKI, R TILLEUX	62	601617
KIN	B N		
	SLEPTSOV, V SAMSON	59	200766
PHAS	B N		
	WENTORF, R	61	700935
PHAS	B N		
	WANG, C	62	301376
VAP	B N		
	HILDENBRAND, D HAL	63	301241
VAP	B N		
	FESENKO, V BOLGAR	63	301216
PREP	B N		
	TAGAWA, H ITOUJI	62	201935
REAC	B N		
	SAMSONOV, G KOVALC	63	900221
REV	B N		
	SAMSONOV, G SEMENO	62	300582
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	MEZAKI, R TILLEUX	62	601617
SPK	B N		
	REDFIELD, D BAUM	61	200978
THEO	B N		
	SAMSONOV, G KOVALC	63	900221
VAP	B N		
	HILDENBRAND, D HAL	63	202050
REAC	B N		
	BOSCH, F	62	202008
THER	B N		
	HILDENBRAND, D L	61	300219
THER	B N		
	FUGET, C R MASI, J	57	300243
TRT	B N		
	THOMAS, J WESTON	62	301039
VAP	B N		
	AKISHIN, P KHODEEV	62	300592
VAP	B N		
	FESENKO, V	62	300711
VAP	B N		
	DREGER, L DADAPE,	62	300604
VAP	B N		
	DREGER, L	62	300720
VAP	B N		
	DREGER, L	61	300528
VAP	B N		
	DREGER, L MARGRAVE	60	600642
VAP	B N		
	JENSEN, A GOSHGART	62	301256
THER	B N SYST		
	SAMSONOV, G	59	201343
ERES	B N SYST		
	SAMSONOV, G	61	601585
PHAS	B N SYST		
	SAMSONOV, G	61	601585
SPK	B O		
	KUZYAKOV, Y TATEVS	60	301065
E	B O		
	LAGERQVIST, A NILS	58	600702
REAC	B O		
	ZINTH, E MORAWIETZ	40	300149
SPK	B O		
	KUZYAKOV, Y TATEVS	60	600694
SPK	B O		
	SINGH, N	49	600703
SPK	B O		
	WELTNER, W WARN, J	62	300588
SPK	B O		
	MALTSEV, A KUZYAKO	57	300316
SPK	B O		
	KASHAR, W ET AL	61	300403
DH	B O 2		
	RUSIN, A TATEVSKII	63	202125
SPK	B O 2		
	JOHNS, J	62	300816
DH	B 2O		
	GALCHENKO, G KORNI	60	700916
SPK	B 2O 2		
	SOMMER, A WHITE, D	63	202141
SPK	B 2O 2		
	SOMMER, A WHITE, D	63	202141
SPK	B 2O 3		
	AKISHIN, P VILKOV	62	301167
SPK	B 2O 3		
	SOMMER, A WHITE, D	63	202141
COPT	B 2O 3		
	MARKIN, E SOBOLEV,	61	700688
CPH	B 2O 3		
	KRASOVITSKAYA, R K	61	700968
CPH	B 2O 3		
	KRASOVITCHAYA, R M	61	300196
CPH	B 2O 3		
	KRASOVITSKAYA, R K	61	300336
CRYS	B 2O 3		
	MACKENZIE, J	61	600882
CRYS	B 2O 3		
	MACKENZIE, J CLAUS	61	700516
DH	B 2O 3		
	BERKOWITZ, J CHUPK	59	700893
DH	B 2O 3		
	GALCHENKO, G KORNI	59	300673
DH	B 2O 3		
	ANON	61	300228
H	B 2O 3		
	KRASOVITSKAYA, R K	61	700968
MSP	B 2O 3		
	BERKOWITZ, J CHUPK	59	700893
PHAS	B 2O 3		
	GIELLISSE, P ROCKE	60	601573
PHAS	B 2O 3		
	MACKENZIE, J CLAUS	61	700516
SPK	B 2O 3		
	LOWRIE, R	61	700956
SPK	B 2O 3		
	TATEVSKII, V KOPTE	61	300384
SPK	B 2O 3		
	MALTSEV, A MATVEEV	61	300949
SPK	B 2O 3		
	MALTSEV, A A TETEV	61	700604
THER	B 2O 3		
	BERKOWITZ, J CHUPK	59	700893
VAP	B 2O 3		
	HILDENBRAND, D HAL	63	301470
VAP	B 2O 3		
	FIRSOVA, L NESEMEY	60	200761
VAP	B 2O 3		
	NESMEYANOV, A FIRS	60	600832
VAP	B 2O 3		
	LOWRIE, R	61	700943
VAP	B 2O 3		
	FIRSOVA, L NESMEYA	60	701004

VAP	B 2O 3	NIKITIN, O AKISHIN	62	300954
VAP	B 2O 3	GIELLISSE, P ROCKE	60	601573
REAC	B 60	RIZZO, H SIMMONS	62	601671
THEO	B O SYST	KROGH-MOE, J	63	301288
THER	B O SYST	MARGRAVE, J	61	301531
SPK	B O SYST	GREENE, F	61	201357
VAP	B O SYST	FIRSOVA, L NESMEYA	60	201020
VAP	B O SYST	NESMEYANOV, A FIRS	59	201019
PHAS	B O SYST	NADOR, B	60	200938
SPK	B O SYST	MATVEEV, V MALTSEV	61	300775
SPK	B O SYST	KASKAN, W MACKENZI	61	600700
VAP	B O SYST	SCHICK, H ANTHROP	63	300994
VAP	B O SYST	SCHICK, H ANTHROP	62	300995
REAC	B O C SYST	RENTZEPIS, P WHITE	59	300971
DH	B O F SYST	FARBER, M	62	201516
THER	B O F SYST	MAGEE, E	61	201511
MSP	B O H SYST	SHOLETTE, W PORTER	63	300988
PHAS	B O H SYST	ABRIKOSOV, N LIANG	60	300848
VAP	B O H SYST	WHITE, D WALSH, P	59	300685
VAP	B O H SYST	ABRIKOSOV, N LIANG	60	300848
MISC	B SI SYST	COLTON, E	61	700609
MPP	B SI SYST	WILLIAMS, E	61	300505
REAC	B SI SYST	COLTON, E	61	700609
CRYS	B SI C SYST	PORTNOI, K SAMSONO	60	300144
ERES	B SI C SYST	PORTNOI, K SAMSONO	60	300144
PHAS	B SI C SYST	PORTNOI, K I SAMSO	60	300144
PHAS	B SI C SYST	MEERSON, G DERGUNO	61	300373
REAC	B SI C SYST	SAMSONOV, G SOLONN	60	200894
SPK	BA	PENKIN, N SHABANOV	62	601601
CEMP	BA B 6	LAFFERTY, J	50	400541
DH	BA O	HOLLOWAY, H	62	300525
DH	BA O	MAH, A	63	202093
E	BA O	LAGERQVIST, A HULD	54	600681
PHAS	BA O	ROTH, R WARING, J	61	201406
REAC	BA O	LEONOV	61	301522
VAP	BA O	NIKONOV, B P OTMAK	61	300254
VAP	BA O	METSON, G	63	301536
DHD	BA OXIDES	VEITS, I GURVICH	56	700964
THER	BA OXIDES	VEITS, I GURVICH,	56	700964

PHAS	BA W O SYST	PURT, G	6?	30[illegible]
BIB	BE	WOHLL, M	60	700723
BIB	BE	ANON	60	700718
REV	BE	SIEMS, P	63	301362
BIB	BE	GUILL, J WORONCOW	59	601580
BIB	BE	CARROLL, K	60	700662
CEMP	BE	CORNWELL, J	61	700667
CPH	BE	JOSHI, S MITRA, S	60	200767
CPH	BE	BEAVER, W OROURKE	59	700933
CPH	BE	KANTOR, P KRASOVIT	60	700955
CPH	BE	WALKER, B EWING, C	62	301098
CPH	BE	KANAZARVA, E PACKE	58	600626
CPH	BE	WILLIAMS, N N	61	700659
CPL	BE	JOSHI, S MITRA, S	60	200767
CRYS	BE	ANON	61	700932
CRYS	BE	BAKAKIN, V BELOV	62	201714
CRYS	BE	FOUNFELKER, R SIET	62	701089
CTEX	BE	BEAVER, W OROURKE	59	700933
CTEX	BE	MEYERHOFF, R SMITH	62	300809
DH	BE	GOLDSMITH, A HIRSC	60	700930
ELCH	BE	PROPIN, R	61	201031
ERES	BE	MARTIN, A BUNCE, J	62	301079
ERES	BE	BRIDGMAN, P	51	400533
H	BE	KANTOR, P KRASOVIT	60	700955
KIN	BE	GREGG, [illegible]	61	201244
MPP	BE	KAUFMANN, A GORDON	50	500129
PHAS	BE	GOLDSMITH, A HIRSC	60	700930
PHAS	BE	PICKETT, J LEVINE	62	601587
PHAS	BE	PAINE, R CARRABINE	60	201197
PHAS	BE	AMONENKO, V IVANOV	62	301124
PHAS	BE	AMONENKO, V IVANOV	61	300535
PHAS	BE	MANNAS, D SMITH, J	62	201786
PMCH	BE	AMONENKO, V PAPIRO	62	300565
REAC	BE	HOOPER, E KEEN, N	60	200947
REAC	BE	BASCHE, M SHETKY	60	201132
REAC	BE	GREGG, S	61	201244
REAC	BE	GREGG, S	61	201133
REAC	BE	DARRAS, R	62	301433
REAC	BE	HIGGINS, J ANTILL	62	201606

REV	BE		
ANON		63	301397
REV	BE		
WOHLL, M		60	701053
REV	BE		
HODGE, W		61	700659
REV	BE		
MOURET, P RIGAUD		58	201527
SPK	BE		
CODLING, K		61	600775
SPK	BE		
JOHANSSON, L		62	601624
SPK	BE		
SHKLVAREVSKII, I		61	201326
SURF	BE		
EREMENKO, V NIZHEN		60	200821
TCON	BE		
BEAVER, W OROURKE		59	700933
THER	BE		
WILLIAMS, N N		61	700659
THER	BE		
BARRIAULT, R DREIK		62	300865
THER	BE		
CHERKASKIN, Y GLAD		57	301107
TRT	BE		
GELLES, S PICKETT		60	600867
VAP	BE		
FRANZEN, J HINTENB		61	700970
VAP	BE		
GOLDSMITH, A HIRSC		60	700930
VAP	BE		
HANLIN, H		60	700951
VAP	BE		
NIKITIN, O GOROKHO		61	700692
PHAS	BE B		
MARKEVICH, G MARKO		60	201315
REAC	BE B 2		
MARKOVSKII, L		62	301530
REAC	BE B 2		
MARKEVICH, G MARKO		60	700937
CRYS	BE B 12		
BECHER, H		60	201128
SPK	BE2		
HAMPSON, R DOOLING		60	201753
REAC	BE4B		
BECHER, H SCHAEFER		62	301405
CRYS	BE5B		
MARKEVICH, G KONDR		60	600630
CRYS	BE B SYST		
SANDS, D E CLINE		61	700566
PHAS	BE B SYST		
HOENING, C CLINE,		61	700691
REAC	BE B SYST		
MARKEVICH, G MARKO		61	700917
PHAS	BE B O SYST		
RASE, D		60	600872
REAC	BE2C		
MARKOVSKII, L		62	301530
THER	BE2C		
SCHICK, H ANTHROP		63	301579
THER	BE2C		
MURATOV, F NOVOSEL		62	601602
ZKP	BE2C		
MURATOV, F S NOVOS		59	300162
CRYS	BE CA		
BAKER, T		62	201513
DH	BE CL2		
THOMPSON, C SINKE		62	201817
MPP	BE COMPOUNDS		
SHUBERT, J		60	701036
REAC	BE COMPOUNDS		
SHUBERT, J		60	701036
PHAS	BE C SYST		
MURATOV, F NOVOSEL		61	300771
REAC	BE F 2		
EVSTYUKHIN, A		59	200852
SPK	BE F 2		
OBUKHOV-DENISOV, V		60	200912
SPK	BE F 2		
KUTYRKIN, V PEIZUL		57	201203
CRYS	BE MG		
BAKER, T		62	201513
PHAS	BE MO SYST		
ARZHANYI, P		59	200822
THER	BE3N 2		
SCHICK, H ANTHROP		63	301560
VAP	BE3N 2		
GREENBAUM, M YATES		62	301231
BIB	BE O		
ANON		61	700925
CPH	BE O		
VICTOR, A DOUGLAS		63	301372
REAC	BE O		
MURATOV, F NOVOSEL		63	301309
REAC	BE O		
KOMAREK, K COUCOUL		63	301269
CPH	BE O		
GREENBAUM, M YATES		62	301231
THER	BE O		
BLAUER, J GREENBAU		63	301190
CPH	BE O		
KANDYBA, V KANTOR		60	700893
CPH	BE O		
WALKER, B EWING, C		62	301098
CRYS	BE O		
AUSTERMAN, S		63	201996
MPP	BE O		
ROTHMANN, A		62	202122
CPH	BE O		
KANDYBA, V V KANTO		60	700533
CPH	BE O		
MAGNUS, A DANZ, H		26	700560
CPL	BE O		
ASLANIAN, J CAILLA		61	201193
CRYS	BE O		
BUDNIKOV, P DELYAE		60	701043
CRYS	BE O		
MILLER, K		60	700952
CRYS	BE O		
KULESHOV, I SADIKO		62	300770
CRYS	BE O		
BUDNIKOV, P SHISHK		61	300470
CRYS	BE O		
SMITH, D CLINE, C		62	701073
CRYS	BE O		
AUSTERMAN, S		62	701072
CRYS	BE O		
AUSTERMAN, S BELIN		63	301127
CRYS	BE O		
BELLAMY, B BAKER		62	201930
CTEX	BE O		
MILLER, K		60	700952
DF	BE O		
BUDNIKOV, P DELYAE		60	701043
DH	BE O		
BUDNIKOV, P DELYAE		60	701043
DH	BE O		
SMIRNOV, M CHUKREE		58	700523
ERES	BE O		
BUDNIKOV, P DELYAE		60	701043
H	BE O		
BUDNIKOV, P DELYAE		60	701043
H	BE O		
RODIGINA, E GOMELS		61	700966
H	BE O		
KANDYBA, V KANTOR		60	700893
KIN	BE O		
NAKATA, M		60	200855
MISC	BE O		
BENTLE, G		62	301130
MPP	BE O		
RILEY, W MCCLELLAN		62	301080
MPP	BE O		
BUDNIKOV, P DELYAE		60	701043
MPP	BE O		
ANON		61	700715

MPP	BE O	GUZMAN, I POLYBOYA	62	300894
MPP	BE O	AUSTERMAN, S	61	201320
PHAS	BE O	ANON	61	700715
PHAS	BE O	BAKER, T BALDOCK,	62	300541
PHAS	BE O	BUDNIKOV, P DELYAE	60	701043
PHAS	BE O	MASSAZZA, F	61	201293
PHAS	BE O	SMITH, D CLINE, C	62	701073
PHAS	BE O	AUSTERMAN, S	62	701072
REAC	BE O	AUSTERMAN, S	63	301400
REAC	BE O	EDWARDS, P HAPPEL	62	301136
SPK	BE O	DURIG, J LORD, C	62	201969
REV	BE O	CHERON, T	61	301429
REV	BE O	BUDNIKOV, P DELYAE	60	701043
SPK	BE O	THRUSH, B	60	200961
SPK	BE O	PARKINSON, W NICHO	59	600612
SPK	BE O	VEITS, I GURVICH	57	600899
TCON	BE O	BUDNIKOV, P DELYAE	60	701043
TCON	BE O	ADAMS, M	54	600961
THER	BE O	KANDYBA, V V KANTO	60	700533
THER	BE O	BUDNIKOV, P DELYAE	60	701043
THER	BE O	BELYKH, L NESMEYAN	59	700918
THER	BE O	ANON	61	700715
THER	BE O	BARRIAULT, R DREIK	62	300865
VAP	BE O	BUDNIKOV, P DELYAE	60	701043
VAP	BE O	BELYKH, L NESMEYAN	59	700916
VAP	BE O	SEMENENKO, K KURDY	61	300838
VAP	BE O	FIRSOVA, L NESMEYA	60	701004
VAP	BE O	FIRSOVA, L NESEMEY	60	200761
PHAS	BE2O3	GIELISSE, P	62	201740
CEMP	BE OXIDES	PALGUEV, S NECEIMI	62	201717
VAP	BE OXIDES	NESMEYANOV, A FIRS	59	201019
VAP	BE OXIDES	FIRSOVA, L NESMEYA	60	201020
REAC	BE O SYST	GREGG, S HUSSEY, R	60	200870
REAC	BE O SI SYST	SUPOVA, E KELER, E	60	201573
PHAS	BE TI O SYST	SHCHEPOCHKINA, N	56	200958
THER	BIMETALLICS	FASOLINO, L	63	301215
THEO	BINARY	GIESSEN, B GRANT	63	301226
THER	BINARY SYST	VECHER, A GERASIMO	63	202151
VAP	BINARY SYST	YARYM-AGAEV, N KOG	62	300700
THEO	BOILING TEMP	RICHARDSON, D	38	700817
THEO	BOND ENERGY	JAFFEE, H ZUNG, V	61	301480
THER	BONDING	SEIGEL, B	63	301380
THEO	BONDS	SEIGEL, S SEIGEL	63	301358
BOOK	BONDS	MORTIMER, C	63	301307
THEO	BONDS	DURAKOV, V BATSANO	61	300753
REV	BOOK	BUNDY, F STRONG, H	62	201719
THER	BOOK	SCHMIDT, E	60	200814
THER	BOOK	SUSHKOV, V	60	200815
THER	BOOK	GERASIMOV, YA KRES	60	300207
CRYS	BORIDES	ARONSSON, B STENBE	59	201388
REAC	BORIDES	KOVALCHENKO, M SAM	60	201044
REAC	BORIDES	MEYERSON, G	55	300571
REV	BORIDES	ARONSSON, B	61	700585
TCON	BORIDES	LVOV S	61	300937
THEO	BORIDES	BURG, A	60	300418
THEO	BORIDES	ROBINS, D	60	600624
THER	BORIDES	MEYERSON, G	55	301122
DH	BORIDES	WILSON, F		300309
CEMP	BORIDES	GOODMAN, P HOMONOF	61	301460
CEMP	BORIDES	SCLAR,N	61	300682
DH	BORIDES	MASLOV, P	63	202099
CEMP	BORIDES	SILVER, A KUSHIDA	63	300987
CRYS	BORIDES	STERN D MCKENNA	60	200830
CRYS	BORIDES	MELINCHKOV, O POVI	62	300947
CRYS	BORIDES	SAMSONOV, G VAINSH	62	300628
CTEX	BORIDES	ZHURAVLEV, N STEPA	61	201272
DHD	BORIDES	SHULISHOVA, O	62	301587
MPP	BORIDES	VAHLDIEK, F MERSOL		301607
MPP	BORIDES	MARKOVSKII, L KOND	57	300941
MPP	BORIDES	MORDIKE, B	60	300503
PHAS	BORIDES	STADELMAIER, H YUN	62	301594
PHAS	BORIDES	PORTNOY, K	60	700944
REAC	BORIDES	LYUTAYA, M NAZARCH	61	[illegible]
REAC	BORIDES	LAFFERTY, J	51	[illegible]
REV	BORIDES	EICK, H	61	301439
MPP	BORIDES	THOMPSON, R	63	202146
ERES	BORIDES	SAMSONOV, G PADERN	62	202127
REAC	BORIDES	MARKOVSKII, L	63	202098

MPP	BORIDES	LVOV, S NEMCHENKO	63	202090
REAC	BORIDES	HOYT, E W CHORNE	60	300246
MISC	BORIDES	STRASHINSKAYA, L	62	201790
MPP	BORIDES	FITZGERALD, L	63	301217
REV	BORIDES	EMRICH, B	62	301182
THER	BORIDES	OLIVER, R BAIER, R	63	301314
PHAS	BORIDES	GORELIK, S ELYVTIN	62	201947
REAC	BORIDES	MARKOVSKII, L VEKS	62	201986
SPK	BORIDES	MIKHALOB, B SHCHEG	62	900213
CRYS	BORIDES-PT METALS	ARONSSON, B RUNDQV	61	300504

C

VAP	C	BAUN, W HODGSON, F	63	202000
CRYS	C	AUST, R DRICKAMER	63	301176
THER	C	ACKERMANN, R THORN	58	601208
BIB	C	NIGHTINGALE, R	62	701071
BIB	C	CHEN, M	62	301428
CEMP	C	SAMSONOV, G NESHPO	59	201052
CEMP	C	GUMENYUK, V LEBEDE	61	700553
CPH	C	RASOR, N MCCLELLAN	60	700984
CPH	C	VICTOR, A	62	300558
CPH	C	RASOR, N MCCLELLAN	60	700896
CPH	C	LUCKS, C DEEM, H	60	601691
CPH	C	WILLIAMS, N N	61	700559
CRYS	C	NIGHTINGALE, R	62	701071
CTEX	C	RASOR, N MCCLELLAN	60	700984
DH	C	BAKER, C KELLY, A	62	300524
DH	C	DAVIS, A	60	600880
DHD	C	LINDHOLN, E	54	600714
DHT	C	BUNDY, F	63	300859
DHT	C	TITOVA, V FUTERG	62	301040
ERES	C	COHAN, N PUGH, D	63	301431
ERES	C	GUMENYUK, V LEBEDE	61	700553
MPP	C	RASOR, N MCCLELLAN	60	700896
MPP	C	KLEIN, C	62	300915
PHAS	C	BUNDY, F	62	300854
PHAS	C	FUNKE, V NOVIKOVA	62	201704
PHAS	C	NIGHTINGALE, R	62	701071
PHAS	C	STRONG, H	61	301599
REAC	C	ENGELKE, J HALDEN	60	201529
SPK	C	COLLIGAN, G GALASS	61	600860
SPK	C	PUGH, H LEES, J B	61	600842
SPK	C	LOWRIE, R	62	601596
SPK	C	PILCHER, G SKINNER	62	301044
TCON	C	RASOR, N MCCLELLAN	60	700984
TCON	C	RASOR, N MCCLELLAN	60	700896
TCON	C	GUMENYUK, V LEBEDE	61	700553
THEO	C	CROWELL, A	62	300701
THER	C	RASOR, N MCCLELLAN	60	200960
THER	C	WILLIAMS, N N	61	700559
THER	C	BARRIAULT, R DREIK	62	300865
VAP	C	COLLIGAN, G GALASS	61	600860
VAP	C	DAVIS, A	60	600880
VAP	C	DOERNENBURG, E HIN	61	700664
VAP	C	KRIEGER, F	62	300931
VAP	C	LOWRIE, R	62	601596
DHD	C 2	BREWER, L HICKS, W	62	300813
DHD	C 2	BREWER, L HICKS, W	62	300813
SPK	C 2	STEELE, D	63	301595
SPK	C 2	LOWRIE, R	62	601596
VAP	C 2	BREWER, L HICKS, W	62	300813
VAP	C 2	BREWER, L HICKS, W	62	300813
VAP	C 2	LOWRIE, R	62	601596
E	C 3	GOUPIL, R	53	600684
REAC	C 3	CABANNES, F	56	300827
SPK	C 3	CABANNES, F	56	301121
SPK	C 3	BREWER, L ENGELKE	62	300797
SPK	C 3	CLEMENTI, E MCLEAN	62	300814
SPK	C 3	BREWER, L ENGELKE	62	300797
SPK	C 3	DORNENBURG, E HINT	61	300467
VAP	C 3	SHPILRAYN, E ASINO	62	300567
SPK	C 4	CLEMENTI, E	61	300615
DH	C N	BERKOWITZ, J	62	301407
SPK	C N	MOORE, C BROIDA, H	57	600687
SPK	C N	KIESS, C	49	600686
SPK	C N	DOUGLAS, A ROUTLEY	54	600682
SPK	C N	DOUGLAS, A	55	600679

SPK	C N	CARROLL, P	56	600677
SPK	C N	PANNETIER, G MARSI	61	600851
DHD	C O	BRACKETT, T	56	600706
DHD	C O	DOUGLAS, A MOLLER	55	600708
DHD	C O	HOWELL, H	49	600712
DHD	C O	TOENNIES, J GREENE	57	600600
SPK	C O	LOEWENSTEIN, E	60	600919
DHD	C O	LINDHOLN, E	54	600714
E	C O	TOBIAS, I FALLON	60	600695
E	C O	ROSENBLUM, B NETHE	57	600723
MPP	C O	ROSENBLUM, B NETHE	58	600724
SPK	C O	HERZBERG, HUGO, T	56	600711
SPK	C O	GOLDBERG, L MULLER	53	600710
SPK	C O	BURRUS, C	58	600707
SPK	C O	BEDARD, F GALLAGHE	53	600705
SPK	C O	BARROW, R GRATZER	56	600704
SPK	C O	RANK, D EASTMAN, D	61	600835
SPK	C O	BARROW, R	61	600777
SPK	C O	MILLS, I THOMPSON	53	600715
SPK	C O	KISHKO, S	60	300796
SPK	C O	ONAKA, R	57	600716
SPK	C O	PALIK, E RAO, K	56	600717
SPK	C O	PLYLER, E ALLEN, N	58	600718
SPK	C O	PLYLER, E BENEDICT	52	600719
SPK	C O	PLYLER, E BLAINE	56	600721
SPK	C O	RANK, D GUENTHER	57	600722
SPK	C O	SUN, N WEISSLER, E	55	600725
SPK	C O	TANAKA, Y JURAA, A	57	600726
SPK	C O	MCCULLOH, K GLOCKL	53	600727
SPK	C O 2	SUN, N WEISSLER, E	55	600725
SPK	C O SYST	KNIPE, R GORDON, A	56	600713
KIN	C O SYST	GULBRANSEN, E	63	301465
MPP	C NI CO SYST	YASUSHI KOJIMA SAN	61	300189
CPH	CA	FAVSTOVA, D IPPOLI	61	201613
PHAS	CA	BEREZHNOI, A KORDY	62	201553
REAC	CA	GREGG, S JEPSON, W	61	201082
REAC	CA	NORMAN, J	60	200868
REAC	CA	KHLEBNIKOV, G SIMA	61	201625
SPK	CA	CODLING, K	61	600775
VAP	CA	KOCHEROV, P GELD	59	300462
CEMP	CA B 6	LAFFERTY, J	50	400541
CEMP	CA B 6	JOHNSON, R DAANE	63	301489
CTEX	CARBIDES	KRIKORIAN, N WALLA	63	202083
CEMP	CARBIDES	BONDARENKO, B ERMA	62	202007
CEMP	CARBIDES	GOODMAN, P HOMONOF	61	301480
CEMP	CARBIDES	KUBASCHENSKI, O	56	601642
THER	CARBIDES	OLIVER, R BAIER, R	63	301314
MPP	CARBIDES	FITZGERALD, L	63	301217
CPH	CARBIDES	KRIKORIAN, O	62	301111
CRYS	CARBIDES	EPPRECHT, W	51	301109
CRYS	CARBIDES	ATOJI, M	61	701070
CRYS	CARBIDES	ATOJI, M	62	201983
CRYS	CARBIDES	KOVALSKII, A	59	201131
CTEX	CARBIDES	BELIKOV, A	60	201066
DF	CARBIDES	ANON	54	400618
MISC	CARBIDES	STRASHINSKAYA, L	62	201790
MPP	CARBIDES	MORDIKE, B	60	300503
PHAS	CARBIDES	KOVALSKII, A	59	201131
PHAS	CARBIDES	GORELIK, S ELYVTIN	62	201947
REAC	CARBIDES	SAMSONOV, G YASINK	61	100180
REAC	CARBIDES	SAMSONOV, G IASINS	61	300340
REAC	CARBIDES	KOPYLOVA, V	61	201305
SPK	CARBIDES	BELIKOV, A	60	201066
SURF	CARBIDES	ZADUMKIN, S	61	201849
TCON	CARBIDES	RUDY, E BENESOVSKY	60	200808
TCON	CARBIDES	LVOV, S	61	300937
THEO	CARBIDES	ROBINS, D	60	600624
THER	CARBIDES	KUBASCHENSKI, O	56	601642
THER	CARBIDES	KUTSEV, V	62	300358
CRYS	CA C 2	ZELDES, H LIVINGST	61	700971
CRYS	CA C 2	VANNERBERG, N	61	201300
CRYS	CA C 2	VANNERBERG, N	62	300596
CRYS	CA C 2	ATOJI, M MEDRUD, R	59	601210
CRYS	CA C 2	ATOJI, M	61	700864
CRYS	CA C 2	TAGAWA, H FUJIMORI	60	201379
CRYS	CA C 2	BREDIG, M	61	201323
KIN	CA C 2	TAGAWA, H SUGAWARA	62	201839
TRT	CA C 2	JUZA, R SCHUSTER	61	600840

CPH	CA F 2	JOSHI, S MITRA, S	60	200767
CPL	CA F 2	JOSHI, S MITRA, S	60	200767
TCON	CA F 2	SLACK, G	61	201125
PHAS	CA MN SI O SYST	GLASSER, F	62	201741
EMF	CA O	BENZ, R WAGNER, C	61	700640
PHAS	CA O	COCCO, A	59	201168
THER	CA O	SCHICK, H ANTHROP	62	300995
TRT	CA O	SCHNEIDER, S	63	301348
REAC	CA O	RYABCHIKOV, I MIKU	62	301336
VAP	CA O	BABELIOWSKY, T BOE	63	301179
VAP	CA O	BABELIOWSKY, T	63	301178
VAP	CA O	BABELIOWSKY, T BOE	62	301128
E	CA O	LAGERQVIST, A HULD	54	600881
ERES	CA O	COCCO, A BARBARIOL	62	301430
MISC	CA O	LADD, M LEE, W	60	201322
MSP	CA O	BABELIOWSKY, T	62	301403
MSP	CA O	BABELIOWSKY, T BOE	62	301128
PHAS	CA O	COCCO, A VIRDIS, P	61	201316
PHAS	CA O	JUZA, R SCHUSTER	61	600840
PHAS	CA O	BRCIC, B GOLIC, L	62	201636
PHAS	CA O	BAKER, E BUTLER, J	62	201794
REAC	CA O	LEONOV, A	61	301522
SPK	CA O	ORTENBERG, F	61	300795
SPK	CA O	ROSEN, B WENIGER	62	301561
SPK	CA O	LAGERQVIST, A	54	600883
SPK	CA O	HULDT, L LAGERQVIS	55	600893
SPK	CA O	HULDT, L LAGERQVIS	56	600894
SPK	CA O	HULTIN, M LAGERQVI	51	600898
SPK	CA O	VEITS, I GURVICH	57	600899
SPK	CA O	GAYDON, A	55	600900
SPK	CA O	LAGERQVIST, A	53	600925
VAP	CA O	METSON, G	63	301536
CPH	CALORIMETRY	WELTY, J WICKS, C	62	301619
CPH	CALORIMETRY	WITTIG, F	61	301624
DH	CALORIMETRY	KOLESOV, V ZENKOV	62	300766
DH	CALORIMETRY	VASILEV, Y SOBOLEV	62	300767
DH	CALORIMETRY	KOSOV, N RIVIN, O	61	400590
THEO	CALORIMETRY	SEMIKIN, I KOSTOGR	61	900223
THEO	CALORIMETRY	BARNER, J	63	301181
THEO	CALORIMETRY	DENCE, W	63	301211
CPH	CALORIMETRY	MITKINA, E	62	301306
THER	CALORIMETRY	SKURATOV, S M	61	300251
DH	CA COMPOUNDS	SHCHUKAREV, S MORO	62	300598
CEMP	CA O SYST	PALGUEV, S NECEIMI	62	201717
DHD	CA O SYST	VEITS, I GURVICH	56	700964
THER	CA O SYST	VEITS, I GURVICH,	56	700964
PHAS	CA O NB SYST	IBRAHIM, M NORMAN	62	201876
EMF	CA SI O SYST	BENZ, R WAGNER, C	61	700640
MPP	CB C	NORTON, J MOWRY, A	49	300157
CRYS	CD	LAWLEY, A	60	200801
CPH	CE	ARAJS, S COLVIN, R	62	300751
CPH	CE	ARAJS, S COLVIN, R	62	301078
CPH	CE	KOENIGSBERG, E KEL	53	601002
CPH	CE	SPEDDING, F MILLER	51	601241
CPH	CE	JAEGER, F BOTTEMA	36	900102
CPL	CE	WILKINSON, M CHILD	61	601412
CPL	CE	GOODMAN, B	52	100208
CPL	CE	PARKINSON, D H SIM	51	400557
CTEX	CE	ANDRES, K	63	301172
CPL	CE	PARKINSON, D ROBER	57	601151
CRYS	CE	SCHUCH, A STURDNAN	50	400518
CRYS	CE	WEINER, R RAYNOR	59	200871
CRYS	CE	MCHARGUE, C YAKEL	60	600646
CTEX	CE	DASHKOVSKII, A SAV	61	201865
DHT	CE	CAVALLERO, U	43	700895
DHT	CE	KOVIMA, T KIKUCHI	53	100183
ERES	CE	JAEGER, F BOTTEMA	36	900102
ERES	CE	JAMES, N LEGNOLD	52	100206
ERES	CE	BRIDGMAN, P	51	400533
ERES	CE	SPEDDING, F DAANE	57	601066
ERES	CE	GOODMAN, B	52	100208
H	CE	SPEDDING, F MILLER	51	601241
MPP	CE	IONOV, N MITTSEV	61	601411
PHAS	CE	WERNER, R RAYNOR	59	601359
PHAS	CE	WILKINSON, M CHILD	61	601412
PHAS	CE	KOVIMA, T KIKUCHI	53	100183
PHAS	CE	SPEDDING, F DAANE	57	601066
PHAS	CE	LIVSHITS, L GENSHA	62	301524

PHAS	CE	LIKHTER, A	57	601492
PHAS	CE	LIKHTER,A RYUBININ	58	601072
PHAS	CE	BEECROFT, R SWENSO	60	600669
PHAS	CE	GONIKBERG, M SHAKH	57	601064
PHAS	CE	COLVIN, R ARAJS, S	61	600875
PHAS	CE	SPEDDING, F DAANE	57	700872
PHAS	CE	VOGEL, R	17	900105
PHAS	CE	CUBICIOTTI, D	49	900104
PHAS	CE	TROMBE, F FOEX, M	44	900118
PHAS	CE	ROLLA, L IANDELLI	43	900103
REAC	CE	LORIERS, J	49	400542
RHO	CE	EICHELBERGER, J	61	601420
SPK	CE	GARSTANG, R	52	100207
SPK	CE	BRIX, P FRANK, H	60	400526
SPK	CE	SMITH, K SPALDING	62	300777
SPK	CE	SCHWARZSCHILD, M	57	601047
SPK	CE	BURBRIDGE, E BURBR	55	601003
SPK	CE	MURAKAWA, K ROSS	61	400556
SPK	CE	GRATTON, L	52	400567
THER	CE	PARKINSON, D H SIM	51	400557
THER	CE	SPEDDING, F H MCKE	60	700570
THER	CE	SCHICK, H ANTHROP	62	300995
TRT	CE	TROMBE, F FOEX, M	44	900118
TRT	CE	ROCHER, Y	62	301559
TRT	CE	JAEGER, F BOTTEMA	36	900102
TRT	CE	GSCHNEIDER, K ELLI	61	202045
TRT	CE	ROLLA, L IANDELLI	43	900103
TRT	CE	CUBICIOTTI, D	49	900104
TRT	CE	GSCHNEIDNER, K ELL	62	301464
TRT	CE	KOVIMA, T KIKUCHI	53	100183
TRT	CE	VOGEL, R	17	900105
VAP	CE	BEAVIS, L	60	600659
REV	CERAMICS	RAMKE, W LATVA, J	63	202121
REV	CERAMICS	RYSHKEWITCH, E	63	301338
BOOK	CERAMICS	KINGIRY, W	60	301263
CRYS	CE B 4	ZALKIN, A TEMPELTO	53	100198
CEMP	CE B 6	SAMSONOV, G PADERN	59	300143
CEMP	CE B 6	LAFFERTY, J	50	400541
COPT	CE B 6	TSAREV, B ILLARION	63	301369
CRYS	CE B 6	ZHDANOV, G ZHURAVL	57	601061
ERES	CE B 6	PADERNO, Y SAMSONO	61	301072
SPK	CE B 6	TRONEVA, N MARCHUK	58	601157
DF	CE C	DANCY, E EVERETT	52	300876
THER	CE CL2	SENDEROFF, S MELLO	61	200930
THER	CE CL3	WALDEN, G SMITH, D	61	201414
VAP	CE CL3	NOVIKOV, G BAEV, A	62	300686
SPK	CE2	BURBRIDGE, G BURBR	54	600937
SPK	CE2	ARROE, H	54	600959
DF	CE C SYST	MCCABE, C	60	600635
PHAS	CE C SYST	WARF, J PALENIK, G	60	600636
THER	CE F 3	WESTRUM, E BEALE	59	600629
REAC	CE N	SAMSONOV, G LYUTAY	63	301340
ERES	CE N	DIDCHENKO, R GORTS	63	301435
MPP	CE N	SAMSONOV, G LYUTAY	62	301572
CRYS	CE N SYST	ANON	61	601376
CRYS	CE N SYST	IANDELLI, A	37	601276
ERES	CE N SYST	DAOU, J	60	600615
PHAS	CE N SYST	EYRING, L SCHULDT	59	600634
VAP	CE O	KULVARSHAYA, B MAS	60	301064
PHAS	CE O	EYRING, L HOLWBERG	62	601590
THER	CE O	SCHICK, H ANTHROP	62	300995
CPH	CE O 2	KUZNETZOV, F A REZ	60	700537
CPL	CE O 2	WESTRUM, E BEALE	61	300350
CPL	CE O 2	WESTRUM, E BEALE	59	600629
DH	CE O 2	MUTHMANN, W WEISS	04	800144
DH	CE O 2	HIRSCH, A	11	900097
ERES	CE O 2	KEVANE, C	62	601467
H	CE O 2	KING, E CHRISTENSE	61	600826
PHAS	CE O 2	BRUNO, M	50	601385
S	CE O 2	KING, E CHRISTENSE	61	600826
SPK	CE O 2	TRONEVA, N MARCHUK	58	601157
THER	CE O 2	WESTRUM, E BEALE	59	600629
CPH	CE2O 3	PANKRATZ, L KELLEY	63	301549
CPH	CE2O 3	KUZNETSOVA, F A RE	61	700600
CPL	CE2O 3	WELLER, W KING, E	63	301617
CPL	CE2O 3	WESTRUM, E BEALE	61	300350
DH	CE2O 3	HUBER, E HOLLEY, C	53	800963
DH	CE2O 3	MAH, A	61	600689

DH	CE2O 3	KUZNETSOV, F REZUK	60	600690
CRYS	CE2O 3	COURTEL, R LORIERS	50	400519
CRYS	CE2O 3	HONIG, J	58	601631
ERES	CE2O 3	HONIG, J	58	601531
PHAS	CE2O 3	BRUNO, M	50	601385
PHAS	CE2O 3	HONIG, J	58	601531
REAC	CE2O 3	LEONOV, A RUDENKO	62	301521
REV	CE2O 3	HONIG, J	58	601531
SPK	CE OXIDES	BRAUER, G GINGERIC	60	300559
REV	CE OXIDES	HONIG, J	58	600827
THER	CE O SYST	KUZNETSOV, F BELYI	61	300665
MISC	CE O SYST	LORIERS, J	49	400542
DH	CE O SYST	BRAUER, K GINGERIC	60	300415
DH	CE O SYST	WALSH, P N DEVER,	61	700642
PHAS	CE O SYST	EYRING, L SCHULDT	59	600634
PHAS	CE O SYST	BRAVER, G GINGERLI	57	600668
VAP	CB O SYST	BRAUER, K GINGERIC	60	300415
REAC	CE SR O SYST	KELER, E GODINA, N	57	600866
ERES	CE ZR O SYST	PALGUEV, S VOLCHEN	60	201074
BIB	CHEMISTRY	HESLOP, R ROBINSON	62	301028
REV	CHEMISTRY	MARGRAVE, J	62	300472
REV	CHEMISTRY	DROWART, J GOLDFIN	62	201917
THEO	CHEMISTRY	HIRSCHFELDER, J	59	301474
DHD	CHLORIDES	FEBER, R	63	301445
PHAS	CO	FUNKE, V NOVIKOVA	62	201704
VAP	CO	SAXER, R	63	301576
VAP	CO	VINTAIKIN, E TOMAS	61	300452
TCON	CO F 2	SLACK, G	61	201126
PHAS	CO MO	FORSYTH, J DALTE	62	201713
CEMP	COMPOUNDS	SAMSONOV, G SINELN	62	201968
CRYS	COMPOUNDS	GLADISHEVSKII, E	61	201880
REAC	COMPOUNDS	NESPHOR, V	58	200896
DK	COMPOUNDS	MAKSIMOVA, I	62	202094
REAC	COMPOUNDS	PAINE, R STONEHOUS	60	201631
DHD	COMPOUNDS	BRADY, P	60	301412
THEO	COMPOUNDS	DROZIN, N	61	300534
THER	CO P+	ORIANI, R MURPHY	62	201864
PHAS	CO TA	DRAGSDORE, R FORGE	62	201712
ERES	CO W C SYST	FUNKE, V SHURSHAKO	61	301453
BIB	CR	WOHLL, M	60	700723
CPH	CR	KRENTSIS, R P	61	300195
CPH	CR	KRAUSS, F	58	700647
CPH	CR	JOHNSON, R	60	301488
CPL	CR	BEAUMONT, R CHIHAR	60	200959
TRT	CR	ALLEN, B MAKKUTH	63	301169
PHAS	CR	GRIGORYEV, A SOKOL	61	301234
TRT	CR	WYDER, W HOCH, M	63	301383
CPL	CR	DEWAR, J	13	700511
CPL	CR	CLUSUIS, K FRANYOS	62	301051
CPL	CR	RICHARDS, T JACKSO	10	700565
CRYS	CR	GRIGOREV, A SOKOLO	61	600653
CTEX	CR	VASYUTINSKII, B KA	61	201416
ERES	CR	BRIDGMAN, P	51	400533
ERES	CR	MARCINKOWSKI, M LI	61	600861
PHAS	CR	EDWARDS, A	60	200948
PHAS	CR	GRIGOREV, A SOKOLO	61	700620
PHAS	CR	MORIN, J	62	601571
REAC	CR	DEUTSCH, N ERVIN	60	500123
REAC	CR	SILCOX, N DILLON	61	201734
REV	CR	WOHLL, M	60	701053
SPK	CR	ROSENZWEIG, N PORT	60	700996
SPK	CR	BONNELLE, C	62	201754
SPK	CR	NEMNONOV, S MENSHI	60	200977
THEO	CR	ROSENZWEIG, N PORT	60	700996
THEO	CR	ROSENZWEIG, N PORT	60	700901
TRT	CR	SVECHNIKOV, V	63	301601
TRT	CR	GRIGOREV, A SOKDOV	61	201437
VAP	CR	CANO, G	62	301423
VAP	CR	GULBRANSEN, E ANDR	61	301074
VAP	CR	GULLBRANSEN, E AND	61	300465
VAP	CR	HANLIN, H	60	700951
VAP	CR	AMONENKO, V KRUGLY	61	300466
VAP	CR	IGNATOV, D LEBEDEV	61	301041
VAP	CR	MIKHAILOV, G PRONI	61	300468
CRYS	CR B	MALINCHKOV, O POVI	62	300948
H	CR B	MEZAKI, R TILLEUX	62	601617
REAC	CR B	MARKOVSKII, L	62	301530
S	CR B	MEZAKI, R TILLEUX	62	601617

MPP	CR B 2	MALYUCHKOV, O POVI	62	202095
CPH	CR B 2	KRESTOVNIKOV, A VE	60	300672
DF	CR B 2	KRESTOVNIKOV, A VE	60	300672
H	CR B 2	MEZAKI, R TILLEUX	62	601617
MPP	CR B 2	SHCHERBAKOV, V VEY	60	300964
PHAS	CR B 2	NESHPOR, V KISLYI	59	700521
REAC	CR B 2	MARKOVSKII, L	62	301530
REAC	CR B 2	KOTSCH, H	60	301509
S	CR B 2	MEZAKI, R TILLEUX	62	601617
THER	CR B 2	BOLGAR, A	61	700938
TRT	CR B 2	NESHPOR, V KISLYI	59	700521
VAP	CR B 2	BOLGAR, A	61	700938
CRYS	CR B 6	EPELBAUM, V SEVAST	60	600800
PHAS	CR B 6	EPELBAUM, V SEVAST	60	600800
REAC	CR2B	MARKOVSKII, L	62	301530
PHAS	CR3B 4	ELFSTROM, M	61	300367
CEMP	CR BORIDES	LVOV, S NEMCHENKO	62	201981
CEMP	CR P SYST	CADEVILLE, M MEYER	62	202013
CPH	CR B SYST	KRESTOUNIKOV, A VE	59	200797
CRYS	CR B SYST	MALYUCHKOV, O POVI	62	300584
CRYS	CR B SYST	EPELBAUM, V SEVAST	57	700931
MPP	CR B SYST	MERZ, A KOTSCH, H	62	301301
PHAS	CR B SYST	EPELBAUM, V SEVAST	57	700931
REAC	CR B SYST	KOLOMYTSEV, P	58	300347
REAC	CR B MO SYST	TAI, S YOSINSKA, G	60	300272
PHAS	CR B P SYST	RUNDQVIST, S	62	300546
PHAS	CR B2 MO SYST	KOVALCHENKO, M SAM	60	300216
PHAS	CR B2 MO SYST	KOVALCHENKO, M SAM	60	300216
CTEX	CR BE	WHITE, G	61	201739
MPP	CR C	KOSOLAPOVA, T SAMS	62	300918
REAC	CR C	KOSOLAPOVA, T SAMS	62	300925
REAC	CR C	SAMSONOV, G KOSOLA	61	300555
VAP	CR3C 2	FESENKO, V BOLGAR	63	301216
CRYS	CR3C 2	MEINHARDT, D KRISE	60	700912
THER	CR3C 2	BOLGAR, A	61	700938
THER	CR3C 2	ANON	60	700992
THER	CR3C 2	ANON	60	700904
THER	CR3C 2	FUJISHIRA, S GOKCE	61	700615
THER	CR3C 2	FUJISHIRO, S GOKCE	61	201015
VAP	CR3C 2	ANON	60	700904
VAP	CR3C 2	BOLGAR, A	61	700938
VAP	CR3C 2	ANON	60	700992
VAP	CR3C 2	ANON	60	600666
CEMP	CR CARBIDES	LVOV, S NEMCHENKO	62	201981
CEMP	CR CARBIDES	LVOV, S NEMCHENKO	61	200968
KIN	CR CARBIDES	KOSOLAPOVA, T SAMS	61	200957
THER	CR CARBONYLS	KAWAI, K MURATA, H	60	200806
DF	CR C SYST	ALEKSEEVA, V	61	300201
REAC	CR C SYST	KOSOPLAPOVA, T SAM	63	301275
DF	CR C SYST	VINTAIKIN, E	63	202155
DF	CR C SYST	ALEKSEEVA, V SHVAR	61	700632
MPP	CR C SYST	BURYLEV, B	61	301071
PHAS	CR CO SYST	GRIGOREV, A YEH, Y	60	201782
PHAS	CR FE SYST	GRIGOREV, A SOKOLO	60	600912
THER	CR FE SYST	KUBASCHEWSKI, O	60	600696
THER	CR FE SYST	WADA, H KAWAI, Y	61	700627
THER	CR MO SYST	LAFFITTE, M KUBASC	61	700626
MPP	CR N	SAMSONOV, G VERKHO	61	301573
VAP	CR N	SANO, K	55	300983
MPP	CR N	SAMSONOV, G VERKHO	62	300997
PHAS	CR NB SYST	MISENCIK, J	60	201432
PHAS	CR NB SYST	PAN, V	61	201635
PHAS	CR NB MO SYST	GOLDSCHMIDT, H BRA	61	201069
PHAS	CR NB MO SYST	KURNAKOV, N TRONEV	60	201338
PHAS	CR NB MO SYST	SVECHNIKOV, V KOBZ	61	201496
PHAS	CR NB SI SYST	GOLDSCHMIDT, H BRA	61	201070
THER	CR NI SYST	KUBASCHEWSHI, O DE	60	300211
PHAS	CR NI NB SYST	SVECHNIKOV, V PAN	61	201495
CEMP	CR NITRIDES	LVOV, S NEMCHENKO	62	201981
CEMP	CR NITRIDES	SAMSONOV, G	60	700947
DH	CR NITRIDES	SAMSONOV, G	60	700947
MISC	CR NITRIDES	POPOVA, U	61	201082
MPP	CR NITRIDES	VERKHOGLYADOVA, T	61	201355
REV	CR NITRIDES	SAMSONOV, G	60	700947
DHD	CR O	HULDT, L LAGERQVIS	52	600764
DHD	CR O	LAGERQVIST, A HULD	53	600765
REAC	CR O	TAKEKAZU, B HIROTA	61	201549
SPK	CR O	BERG, R SIMANOGLN	60	301089

THER	CR O	BARRIAULT, R DREIK	62	300865
CRYS	CR O 2	CLOUD, W SCHREIBER	62	201931
MPP	CR O 2	SWABODA, T ARTHUR	61	700524
DK	CR O 2	KUBATA, B	61	700586
REAC	CR O 2	KUBATA, B	61	700586
THER	CR O 2	KUBATA, B	61	700586
THER	CR O 2	BARRIAULT, R DREIK	62	300865
S	CR O 3	SPITSYN, V AFONSKI	60	300819
THER	CR O 3	BARRIAULT, R DREIK	62	300865
CRYS	CR2O 3	GRAHAM, J	60	h 600818
DF	CR2O 3	JEANNIN, Y MANNERS	63	301483
PHAS	CR2O 3	JAFFRAY, J	61	700655
REAC	CR2O 3	SAMSONOV, G KOSOLA	61	300555
TRT	CR2O 3	MCNALLY, R PETERS	61	600826
VAP	CR2O 3	WANG, K DREGER, L	60	700897
VAP	CR2O 3	CAPLAN, D COHEN, M	61	700529
VAP	CR2O 3	KE CHING WONG DREG	60	300140
VAP	CR2O 5	NEUGENAUER, J	63	301311
REAC	CR3O	KIHLBORG, L	62	202068
MISC	CR OXIDES	LUX, H EBERLE, L	61	700628
PHAS	CR OXIDES	ANDERSSON, S	59	201178
PHAS	CR O SYST	KUBOTA, T	61	600910
VAP	CR O SYST	GLEMSER, O MUELLER	62	300759
PHAS	CR RU SYST	SAVITSKII, E TEREK	61	300836
MISC	CR SALTS	LUX, H EBERLE, L	61	700628
CPH	CR SI SYST	GOLUTVIN, U LYAN	61	700540
DH	CR SI SYST	GOLUTVIN, V LYAN	61	700540
DH	CR SI SYST	GOLUTVIN, Y	62	301229
H	CR SI SYST	GOLUTVIN, U LYAN	61	700540
THER	CR SI SYST	GOLUTVIN, U LYAN	61	700540
THEO	CRYSTAL	DOYAL, B	61	300223
PHAS	CR TA SYST	GRIGOREV, A SOKDOU	60	201646
THER	CR TA SYST	PILOYAN, G O EVSEE	60	300178
THER	CR TA SYST	PILOYAN, G EVSEEV	60	600688
PHAS	CR U O SYST	SMITH, D CLEIN, C	61	201483
PHAS	CS NB O SYST	REISMAN, A MINEO	61	201080
BIB	CU	RICHERT, E BECKETT	49	700564
DH	CU	VERHAEGEN, G		300235
MPP	CU	RICHERT, E BECKETT	49	700564
REV	CU	RICHERT, E BECKETT	49	700564

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THEO	DIATOMIC GASES	GUNGMAN, V	61	700548
THEO	DIATOMIC GASES	ARAI, T	60	300842
THER	DIATOMIC GASES	BROUNSHTEIN, B YUR	62	300774
THER	DIATOMIC GASES	GURVICH, L YUNGMAN	60	300460
DHD	DIATOMIC MOLECULE	SAYASOV, Y IVANOV	60	400593
REV	DIATOMIC MOLECULE	HERZBERG, G	52	600536
SPK	DIATOMIC MOLECULE	HOUGEN, J	62	300784
SPK	DIATOMIC MOLECULE	FOGARASSY, B NEMET	60	200879
SPK	DIATOMIC MOLECULE	HERZBERG, G	52	600536
THEO	DIATOMIC MOLECULE	BROUNSHTEIN, B I	61	300187
THEO	DIATOMIC MOLECULE	PAPOUSEK, D	61	700676
THEO	DIATOMIC MOLECULE	LIPPINCOTT, E STEE	61	700683
SPK	DIATOMIC,1ST ROW	FROGA, S RANAIL, B	61	700644
THEO	DIATOMICS	VANDERSLICE, J	62	202150
SPK	DIATOMICS	NIKITIN, E	62	301312
DHD	DIATOMICS	PRITCHARD, H	62	301554
DHD	DIATOMICS	CLEMENTI, E	63	301204
SPK	DIATOMICS	JENSOVSKY, L	62	301487
THEO	DIATOMICS	RUE, R	63	301335
THEO	DIATOMICS	RICE, O	62	301557
THEO	DIATOMICS	SPIRIDONOV, V TATE	61	301592
THER	DIATOMICS	PAPOUSEK, D CERMAN	62	301550
MISC	DIBORIDES	MARKOVSKII, L VEKS	61	201060
THEO	DIFFRACTION	RAMBIDI, N SPIRIDO	62	301389
CEMP	DY	LEGVOLD, S SPEDDIN	53	100189
CPL	DY	DREYFUS, B	61	201220
CPL	DY	GRIFFEL, M	56	601263
CPL	DY	LOUNASMAA, O GUENT	62	300779
CPL	DY	GRIFFEL, M SKOCHDO	56	601018
CRYS	DY	KOEHLER, W WOLLAN	61	301504
CRYS	DY	FOUNFELKER, R SIET	62	701069
DH	DY	HUBER, E	56	601291
DH	DY	SAVAGE, W HUDSON	59	601126
DH	DY	WHITE, D	61	201217
ERES	DY	COLVIN, R LEGVOLD	60	601389

ERES	DY		
	LEGUOLD, S SPEDDIN	53	100189
ERES	DY		
	COLES, B	58	601498
SPK	DY		
	DONTSOV, Y	56	601055
REAC	DY		
	OLCESE, G	61	201602
SPK	DY		
	AKIMOV, A	57	601099
SPK	DY		
	MERRILL, P GREENST	56	601007
SPK	DY		
	SMITH, K SPALDING	62	300777
CRYS	DY		
	DARNELL, F MOORE,E	63	202023
SPK	DY		
	BURBRIDGE, E BURBR	55	601003
SPK	DY		
	MURAKAWA, K KAMEI	53	601218
VAP	DY		
	WHITE, D WALSH, P	60	301622
VAP	DY		
	WHITE, D WALSH, P	61	300455
VAP	DY		
	SAVAGE, W HUDSON	59	601126
CEMP	DY B 6		
	SAMSONOV, G PADERN	59	300143
VAP	DY O		
	KULVARSHAYA, B MAS	60	301064
SPK	DY2		
	BURBRIDGE, G BURBR	54	600937
CPL	DY2O 3		
	WESTRUM E JUSTICE	63	301012
CPH	DY2O 3		
	PANKRATZ, L KELLEY	63	301549
CRYS	DY2O 3		
	STARITZKY, E	56	601292
CTEX	DY2O 3		
	PLOETZ, G	57	601309
DH	DY2O 3		
	HUBER, E	56	601291
PHAS	DY2O 3		
	STARITZKY, E	56	601030

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THEO	EFFUSION		
	PRISELKOV, Y SAPOZ	60	300423
THEO	EFFUSION		
	FIRSOVA, L	62	301448
THEO	EFFUSION		
	SEARCY, A SCHULZ	63	300980
CPL	EINSTEIN FUNCTION		
	OVERTON, W C HANCO	60	300244
BETA	ELEMENTS		
	EGYED	54	700739
CPL	ELEMENTS		
	SKIFFMAN, C	62	601636
DH	ELEMENTS		
	NESMEYANOV, A KHAN	60	600660
REAC	ELEMENTS		
	RYABCHIKOV, D SKLY	60	200787
REAC	ELEMENTS		
	ROLSTEN, R	60	200786
REV	ELEMENTS		
	SHARPE, A SHARP, D	61	201631
SPK	ELEMENTS		
	WATSON, R	60	200816
THER	ELEMENTS		
	GATES, D THODOS, G	60	201372
VAP	ELEMENTS		
	ORMONT, B	62	300765
VAP	ELEMENTS		
	NESMEYANOV, A	61	300422
VAP	ELEMENTS		
	HONIG, R	62	301144
ERES	ELEMENTS, GROUP 2		
	VOROBER, A NAKHODN	58	201600
REAC	ELEMENTS, GROUP 4		
	CHIANG, T	62	201680
THEO	ENTROPY		
	DROZIN, N	61	300668
THEO	EQUILIBRIUM		
	POE, A	63	301551
CEMP	ER		
	LEGVOLD, S SPEDDIN	53	100189
CRYS	ER		
	KOEHLER, W WOLLAN	61	301504
DH	ER		
	TRULSON, O HUDSON	61	600832
DH	ER		
	WHITE, D	61	201217
ERES	ER		
	COLVIN, R LEGVOLD	60	601389
ERES	ER		
	LEGUOLD, S SPEDDIN	53	100189
ERES	ER		
	COLES, B	58	601498
MPP	ER		
	IONOV, N MITTSEV	61	601411
SPK	ER		
	SMITH, K SPALDING	62	300777
SPK	ER		
	JUDD, B MARQUET, L	62	300801
SPK	ER		
	AKIMOV, A	57	601099
VAP	ER		
	WHITE, D WALSH, P	60	301622
VAP	ER		
	WHITE, D WALSH, P	61	300455
CEMP	ER B 6		
	SAMSONOV, G PADERN	59	300143
VAP	ER O		
	KULVARSHAYA, B MAS	60	301064
CPL	ER2O 3		
	WESTRUM, E JUSTICE	63	301012
CPH	ER2O 3		
	PANKRATZ, L KING	63	202114
PHAS	ER2O 3		
	STARITZKY, E	56	601030
DH	EU		
	TRULSON, O HUDSON	61	600832
ERES	EU		
	OLSEN, C	60	601336
PHAS	EU		
	COLVIN, R ARAJS, S	61	600875
PHAS	EU IN O SYST		
	SCHNEIDER, S	61	201537
SPK	EU		
	SAKELLARIDIS, P	53	100164
SPK	EU		
	VAN DIJKE BEATTY, S	51	400548
SPH	EU		
	BRIX, P	52	400566
SPK	EU		
	BURBRIDGE, E BURBR	55	601003
SPK	EU		
	MERRILL, P GREENST	56	601007
SPK	EU		
	BRIX, P KOPPERMAN	52	400574
SPK	EU		
	BOHM VITENSE, E	60	601169
CEMP	EU B 6		
	SAMSONOV, G PADERN	59	300143
CRYS	EU B 6		
	FELTEN, E BENDER	58	700867
CRYS	EU N		
	EICK, H BAENZIGER	56	601046
PHAS	EU N		
	EICK, H BAENZIGER	56	601046
REAC	EU N		
	EICK, H BAENZIGER	56	601046

REAC	EU NITRIDES		
	EICK, H	57	601053
VAP	EU O		
	KULVARSHAYA, B MAS	60	301084
SPK	EU2		
	BURBRIDGE, G BURBR	54	600937
CTEX	EU2O 3		
	PLOETZ, G	57	601309
MPP	EU2O 3		
	CURTIS, C THARP, A	59	700804
MSP	EU2O 3		
	PANISH, M	61	601372
TRT	EU2O 3		
	WISNYI, L PIJANOWS	57	601056
VAP	EU2O 3		
	PANISH, M	61	601372
CRYS	EU3O 4		
	BAERNIGHAUSEN, H	62	701088
SPK	EUII		
	DEUTSCH, A	56	600982
BIB	EU OXIDES		
	JONES, P	60	200984
PHAS	EU OXIDES		
	EICK, H BAENZIGER	56	601070
REAC	EU OXIDES		
	EICK, H	57	601053
REAC	EU OXIDES		
	EICK, H BAENZIGER	56	601070
MSP	EXPERIMENTAL		
	LEHRLE, R	62	301520
MSP	EXPERIMENTAL		
	MCDOWELL, C	62	201370
SPK	EXPERIMENTAL		
	HEXTES, R	63	301240

F

BETA	FE		
	KRUPNIKOU, K BAKAN	63	301149
THER	FE		
	KINNE, G VISHKAREV	62	301147
VAP	FE		
	FRANZEN, J HINTENB	61	700970
MPP	FE C SYST		
	MORI, T AKETA, D	60	300205
THER	FE C SYST		
	TSENG, C POLYAKOV	61	301003
THER	FE CO SYST		
	SATO, T KACHI, S	56	300268
PHAS	FE CR SYST		
	WADA, H KAWAI, Y	60	300289
DHD	FE O		
	LAGERQVIST, A HULD	53	600765
PHAS	FE SI B SYST		
	ARONSSON, B ENGSTR	60	201348
MPP	FE SI SYST		
	DRETZE, H D BALTHE	61	300242
PHAS	FE TI C SYST		
	PENG, R CHOV, Y	58	300269
THEO	FUSION		
	FERRIER, A	62	300791
THEO	FUSION		
	GROSSE, A LENTNER	62	300578

G

DH	GA		
	GURVICH, L	60	600652
DHD	GAS METAL DIOXIDE		
	BREWER, L ROSENBLA	61	700957
F	GAS METAL DIOXIDE		
	BREWER, L ROSENBLA	61	700957
SPK	GAS METAL DIOXIDE		
	BREWER, L ROSENBLA	61	700957
F	GASEOUS ATOMS		
	KATZ, T MARGRAVE	55	600933
THER	GASEOUS IONS		
	GREEN, J POLAND, D	60	200782
REV	GASES		
	GLUSHKO, V	62	301221
THEO	GASES		
	HIRSCHFELDER, J CU	54	202061
THEO	GASES		
	HIRSCHFELDER, J	63	202062
BOOK	GASES		
	PENNER, S	62	202117
THER	GASES		
	MCDOWELL, R	63	301300
THEO	GASES		
	PREDVODITELEV, A	63	301322
THER	GASES		
	SEIGEL, B	63	301359
DHD	GASES		
	MATLOW, S	61	300401
DHD	GASES		
	LIPPINCOTT, E ET A	61	300402
SPK	GASES		
	OPPENHEIM, I HAFEM	63	301316
MSP	GASES		
	MARTYNKEVICH, G	62	300357
SPK	GASES		
	HOUGEN, J	62	301479
SPK	GASES		
	WATANABE, K INN, E	52	600565
THEO	GASES		
	GURVICH, L YUNGMAN	61	300354
THEO	GASES		
	BROUNSHTEIN, B YUR	62	300364
THEO	GASES		
	WATANABE, K INN, E	52	600565
THEO	GASES		
	GODNEV, I ALEKASAN	62	300893
THEO	GASES		
	VUKALOVICH, M ARTY	62	301005
THEO	GASES		
	ALTUNIN, V	62	301395
THER	GASES		
	SMITH, F	63	301590
THER	GASES		
	BROUNSHTEIN, B YUR	62	301417
THER	GASES		
	GURVICH, L V YUNGM	61	300248
THER	GASES		
	BAIBUZ, V MEDVEDEV	61	300644
THER	GASES		
	LAVROV, N FILIPPOV	59	300341
THER	GASES		
	KOLSKY, H GILMER,	57	700838
THER	GASES		
	TABACHENKO, A	62	900227
VAP	GASES		
	GILLES, P	62	301142
VAP	GASES		
	HONIG, R HOOK, H	60	300424
VAP	GA O		
	KULVARSHAYA, B MAS	60	301084
VAP	GA O		
	SHCHUKAREV, S SEME	61	300837
CEMP	GD		
	LEGVOLD, S SPEDDIN	53	100189
CPL	GD		
	LOUNASMAA,	63	301527
CPL	GD		
	CRANE, L	62	300811
CRYS	GD		
	FOUNFELKER, R SIET	62	701089
DH	GD		
	TRULSON, O HUDSON	61	600832
CTEX	GD		
	ANDRES, K	63	301172

DH	GD	WHITE, D	61	201217
ERES	GD	COLVIN, R LEGVOLD,	60	601369
ERES	GD	LEGVOLD, S SPEDDIN	53	100189
ERES	GD	COLES, B	58	601498
SPK	GD	MURAKAWA, K	54	601284
SPK	GD	SMITH, K SPALDING,	62	300777
SPK	GD	AKIMOV, A	57	601099
SPK	GD	BUX, P ENGLER, H	52	100192
SPK	GD	ZELDES, N	53	100191
SPK	GD	BURBRIDGE, E BURBR	55	601003
SPK	GD	MERRILL, P GREENST	56	601007
SPK	GD	SUWA, S	53	100190
SPK	GD	SAKELLARIDIS, P	53	100184
SPK	GD	RUSSELL, H	50	400540
SPK	GD	BRIX, P ENGLER, D	51	400563
SPK	GD	BRIX, P	52	400566
SPK	GD	GRATTON, L	52	400567
SPK	GD	SUWA, S	52	400575
VAP	GD	WHITE, D WALSH, P	60	301622
VAP	GD	WHITE, D WALSH, P	61	300455
CRYS	GD B 4	STEPANOVA, A ZHURA	58	601111
CTEX	GD B 4	STEPANOVA, A ZHURA	58	601111
CEMP	GD B 6	SAMSONOV, G PADERN	59	300143
SPK	GD2	BURBRIDGE, G BURBR	54	600937
CPH	GD2O 3	PANKRATZ, L KING	62	300958
CPL	GD2O 3	JUSTICE, B WESTRUM	63	300907
CTEX	GD2O 3	PLOETZ, G	57	601309
DH	GD2O 3	HUBER, E HOLLEY, C	55	600930
REAC	GD2O 3	KELER, E GODINA, N	61	300387
TRT	GD2O 3	WISNYI, L PIJANOWS	57	601056
SPK	GDII	DEUTSCH, A	56	600982
BIB	GD OXIDES	JONES, P	60	200984
CEMP	GE	UNY, C	61	301036
MSP	GE	KOYLOVSKAYA, V		301103
THER	GE	CHERKASKIN, Y GLAD	57	301107
VAP	GE	VINTAIKIN, E	61	201208
DH	GE C SYST	SCACE, R SLACK, G	60	200768
PHAS	GE C SYST	SCACE, R SLACK, G	60	200768
PHAS	GE O	BREWER, L MASTIK	49	601634
MSP	GROUP III-IV-V	AHEARN, A THURMOND	62	300471
THER	GROUP IV-V-VI			

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		HOCH, M	62	300544
REAC	HARD METALS	DEMPSEY, E	63	301134
REAC	HAFNATES	KOMMISSAROVA, L SP	63	202078
THER	HALIDES	BREWER, L SOMAYAJU	63	202010
DH	HALIDES	BARBER, M LINNETT	62	300702
REV	HALIDES	BREWER, L SOMAYAJU	63	301415
RHO	HALIDES	KIRSCHENBAUM, A CA	60	200897
THEO	HEAT CAPACITY	HILSENRATH, J ZIEG	62	301471
THEO	HEAT CAPACITY	FLINN, P MARADUDIN	63	301218
THEO	HEAT CAPACITY	LANDIIA, N	62	301291
CTEX	HEXABORIDES	ZHURAVLEV, N ET AL	61	300379
PHAS	HF	BABITZKE, H ASAI	62	201986
KIN	HF	KUBASCHEWSKI, O	62	601577
THER	HF	KUBASCHEWSKI, O	62	601577
BIB	HF	ABSHIRE, E NOTESTI	60	600649
BIB	HF	CURTIS, C	52	600903
BIB	HF	WILLIAMS, G BAKER	52	600904
CPH	HF	FIELDHOUSE, I LANG	60	601583
CRYS	HF	GLADYSHEVSKII, E TY	60	201564
CRYS	HF	FOUNFELKER, R SIET	62	701089
CTEX	HF	FIELDHOUSE, I LANG	60	601583
CTEX	HF	NOWOTNY, H LAUBE	61	600844
MPP	HF	KAREV, V KLYUCHARE	63	202084
MISC	HF	SPINK, D	61	200891
MPP	HF	SKINNER, G BECKETT	60	601225
PHAS	HF	KORNILOV, I	60	200907
PHAS	HF	MARTIN, R SEAGLE	61	300308
PHAS	HF	NOWOTNY, H BRAUN	60	201309
REAC	HF	ENGELKE, J HALDEN	60	201529
CRYS	HF	JAMIESON, J	63	301253
CPL	HF	KNIEF, G BETTERTON	63	301264
VAP	HF	KRIKORIAN, O	63	301284
REV	HF	SPERNER, H	62	201787
SPK	HF	KLINKENBERG, P	61	300776
SPK	HF	MOORE, C	58	601088

SPK	HF	NORRIS, J	60	601194
SPK	HF	ROSENZWEIG, N PORT	60	700901
SPK	HF	ROSENZWEIG, N PORT	60	700996
SPK	HF	SHAW, C	55	600908
TCON	HF	FIELDHOUSE, I LANG	60	601583
THEO	HF	ROSENZWEIG, N PORT	60	700996
THEO	HF	ROSENZWEIG, N PORT	60	700901
THER	HF	MARGRAVE, J	61	700967
THER	HF	SCHICK, H ANTHROP	63	300994
TRT	HF	TAYLOR, A DOYLE, N	61	600833
TRT	HF	GIESSEN, B RUMP, I	63	301455
TRT	HF	MARTIN, R SEAGLE	61	300308
TRT	HF	GRESSEN, B RUMP, I	62	300887
VAP	HF	PANISH, M REIF, L	63	300959
SPK	HF3	KLINKENBERG, P VAN	61	701019
SPK	HF4	KLINKENBERG, P VAN	61	701019
CEMP	HF B 2	MATSKEVICH, T KAZA	62	300952
CRYS	HF B 2	RUDY, E	61	201255
H	HF B 2	MEZAKI, R TILLEUX	62	601617
KIN	HF B 2	ANON	62	601597
MPP	HF B 2	PADERNO, Y B SEREL	59	700534
REAC	HF B 2	PADERNO, Y B SEREL	59	700534
S	HF B 2	MEZAKI, R TILLEUX	62	601617
THER	HF B 2	LITTLE, A	62	301526
VAP	HF B 2	KRUPKA, M	62	601598
PHAS	HF B C SYST	NOWOTNY, H	61	201147
PHAS	HF B C SYST	NOWOTNY, H RUDY, E	61	300190
PHAS	HF B N SYST	RUDY, E BENESOVSKY	61	300486
PHAS	HF BA O SYST	KELER, E GODINA, N	61	201214
PHAS	HF BE SYST	KRIPYAKEVICH, P TY	61	201377
PHAS	HF B X	VICKERY, R C MUIR	60	300232
TRT	HF B X	VICKERY, R MIUR, H	60	300232
CEMP	HF C	MATSKEVICH, T KAZA	62	300952
CEMP	HF C	BONDARENKO, B ERMA	62	301409
COPT	HF C	COFFMAN, J COULSON	61	701040
CPH	HF C	LOWRIE, R	60	701014
CRYS	HF C	COFFMAN, J COULSON	61	701040
CRYS	HF C	BENESOVSKY, F RUDY	60	700974
DF	HF C	COFFMAN, J COULSON	61	701040
DHD	HF C	BITTNER, H GORETZK	62	301132
MPP	HF C	ANON	61	300237
MPP	HF C	SAMSONOV, G	59	300996
MPP	HF C	SAMSONOV, G PADERN	61	201143
PHAS	HF C	ANON	61	601599
PHAS	HF C	BENESOVSKY, F RUDY	60	700974
MPP	HF C	PADERNO, V	62	202112
CEMP	HF C	SAMSONOV, G FOMENK	63	202128
CEMP	HF C	BITTNER, H GORETZK	62	202004
CEMP	HF C	INGOLD, J	63	301251
CTEX	HF C	KRIHORIAM, WALLA	63	301285
PHAS	HF C	COFFMAN, J COULSON	61	701040
PHAS	HF C	BENESOVSKY, E RUDY	61	100181
PHAS	HF C	CURTIS, C DONEY, L	54	300867
REAC	HF C	MEERSON, G KREIN	60	200831
REAC	HF C	CALVERT, E KIRK, M	62	301421
REAC	HF C	SAMSONOV, G PADERN	61	201143
REAC	HF C	ZHELANKIN, V KUTSE	62	201911
TCON	HF C	LOWRIE, R	60	701014
THER	HF C	BOLGAR, A	61	700938
THER	HF C	SCHICK, H ANTHROP	63	301579
THER	HF C	LITTLE, A	62	301526
VAP	HF C	VIDALE, G	61	301611
VAP	HF C	BOLGAR, A	61	700938
VAP	HF C	COFFMAN, J COULSON	61	701040
VAP	HF C	COFFMAN, J COULSON	61	300293
VAP	HF C	SCHICK, H ANTHROP	63	300994
PHAS	HF C SYST	BENESOVSKY, F RUDY	60	600648
PHAS	HF C SYST	AVARDE, R AUGUSTIN	62	300850
REAC	HF C O SYST	ZHELANKIN, V KUTSE	61	300557
PHAS	HF CA OXIDES	GODINA, N KELER, E	61	201336
SURF	HF CARBIDES	FOMENKO, V	61	201420
PHAS	HF CA O SYST	KELER, E GODINA, N	61	201214
VAP	HF CL 4	TOIRELNIKOV, V KOM	61	301101
VAP	HF CL 4	EVSTYUKHIN, A BARI	60	300882
THER	HF CL SYST	RUZINOV, L BELOV		301568
CEMP	HF COMPOUNDS	LEWIS, C R	61	300234
DH	HF F 4	GREENBERG, E SETTL	62	300739
SPK	HF HALIDES	BUCHLER, A	60	201465

THER	HF HALIDES		
	LUNGU, S	62	300736
PHAS	HF MG O SYST		
	GODINA, N KELER, E	61	201336
PHAS	HF MO SYST		
	KAUFMANN, A RAPPER	60	202065
PHAS	HF MO SYST		
	KAUFMANN A R RAPPR	61	300218
THEO	HF N		
	BAUGHAN, E	59	300868
MPP	HF N		
	SAMSONOV, G VERKHO	62	300997
MPP	HF N		
	SAMSONOV, G	59	300996
CEMP	HF NITRIDES		
	SAMSONOV, G	60	700947
DH	HF NITRIDES		
	SAMSONOV, G	60	700947
rev	HF NITRIDES		
	SAMSONOV, G	60	700947
PHAS	HF O		
	KORNILOV, I	60	200769
THER	HF O		
	SCHICK, H ANTHROP	63	301579
VAP	HF O		
	PANISH, M REIF, L	63	300959
CEMP	HF O 2		
	MATSKEVICH, T KAZA	62	300962
CRYS	HF O 2		
	ADAM, J ROGERS, M	59	300852
CTEX	HF O 2		
	GRAIN, C CAMPBELL	61	601471
PHAS	HF O 2		
	DELIMARSKY, Y BUDE	62	300880
VAP	HF O 2		
	SHCHUKAREV, S SEME	63	301352
PHAS	HF O 2		
	KELER, E GODINA, N	61	300264
PHAS	HF O 2		
	CURTIS, C DONEY, L	54	300867
PHAS	HF O 2		
	GRAIN, C CAMPBELL	61	601471
REAC	HF O 2		
	MCTAGGART, F	61	300338
TRT	HF O 2		
	WOLTEN, G	63	202161
CRYS	HF O 2		
	KOFSTAD, P RUZICKA	63	202073
MPP	HF O 2		
	MCTAGGART, F	63	202101
THER	HF O 2		
	SCHICK, H ANTHROP	63	301580
PHAS	HF O 2		
	LEFEVRE, J	63	301519
THER	HF O 2		
	SCHICK, H ANTHROP	63	301579
TRT	HF O 2		
	BAUN, W	63	201999
THER	HF O 2		
	MCCLAINE, L	60	300278
TRT	HF O 2		
	CURTIS, C DONEY, L	54	300867
VAP	HF O 2		
	HASAPIS, A MELVEGE	61	701017
VAP	HF O 2		
	HASAPIS, A MELVEGE	61	701039
PHAS	HF O SYST		
	RUDY, E STECHER, P	63	300974
PHAS	HF O SYST		
	KUBASCHEWSKI, O	62	601577
THER	HF O SYST		
	SILVER, M FARRAR	63	202137
CRYS	HF O SYST		
	DAGERHAMN, T	61	300478
THER	HF O SYST		
	VEINBACHS, A KOMAR	62	601611
MPP	HF O F SYST		
	BUSLAYEV, Y GORBUN	62	300830
CRYS	HF P		
	JEITSCHKO, W NOWOT	62	301484
PHAS	HF RE SYST		
	SAVITSKII, E TYLKI	62	201795
PHAS	HF RE SYST		
	KAUFMANN A R RAPPR	61	300218
PHAS	HF SR O SYST		
	KELER, E GODINA, N	61	201214
PHAS	HF TA C SYST		
	NOWOTNY, H	63	301165
PHAS	HF TI O SYST		
	GODINA, N KELER, E	60	201522
PHAS	HF U C SYST		
	KRIKORIAN, N WITTE	63	301513
PHAS	HF U C SYST		
	BENESOVSKY, F RUDY	61	301406
PHAS	HF W		
	KAUFMANN A R RAPPR	61	300218
THER	HF X 4		
	ALEKSANDROVSKAYA, A	63	301393
SPK	HG		
	MCNALLY, J	52	100211
REV	HIGH TEMP CHEM		
	GILLES, P	61	300450
CRYS	HO		
	KOEHLER, W WOLLAN	61	301504
CPL	HO		
	LOUNASMAA, O	62	701077
DH	HO		
	WHITE, D	61	201217
ERES	HO		
	COLVIN, R LEGVOLD	60	601389
SPK	HO		
	SAKELLARIDIS, P	53	100184
VAP	HO		
	WHITE, D WALSH, P	60	301622
VAP	HO		
	DEMARIA, G GUIDO	63	202097
VAP	HO		
	WHITE, D WALSH, P	61	301014
VAP	HO		
	WAKEFIELD, G	62	300724
VAP	HO O		
	KULVARSHAYA, B MAS	60	301064
CRYS	HO B 4		
	STEPANOVA, A ZHURA	58	601111
CTEX	HO B 4		
	STEPANOVA, A ZHURA	58	601111
CEMP	HO B 6		
	SAMSONOV G PADERN	59	300143
CPH	HO2O 3		
	PANKRATZ, L KING	63	202114
CPL	HO2O 3		
	WESTRUM, E JUSTICE	63	301012
REV	H. T RESEARCH		
	GROSSE, A	63	301236

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CPH	IN		
	CARTER, W	61	601631
CTEX	IN		
	CARTER, W	61	601631
THER	IN		
	CARTER, W	61	601631
DH	INORGANIC COMPDS		
	REZNITSKII, L A	61	300250
SPK	INORGANIC COMPDS		
	OZIMOV, B VOLNOV	61	700591
DH	INORGANIC SALTS		
	KARPACHEV, S V KAR	60	300138
THER	INORGANIC SALTS		
	KARPACHEV, S V KAR	60	300138
S	INORGANIC SUBSTAN		
	ACKERMANN, R J THO	58	300255

MPP	INTERMETALLICS		
	KOROLKOV, A IGUMNO	61	300536
REV	INTERMETALLICS		
	PAINE, R STONEHOUS	60	201391
REAC	IONS		
	TALROZE, V	60	601643
THER	IONS		
	GREEN, J POLAND, D	62	300353
THER	IONS		
	GREEN, J POLAND, D	61	301462
BIB	IR		
	GOODWIN, T	56	601547
CEMP	IR		
	WHITE, G WOODS, S	57	601050
CPH	IR		
	DOUGLASS, R HOLDEN	59	700375
CPL	IR		
	JOHNSON, R HUDSON	56	601039
CRYS	IR		
	MCCALDIN, J DUWEZ	54	600956
CRYS	IR		
	THOMPSON J	62	201648
DH	IR		
	PANISH, M REIF, L	61	700639
DH	IR		
	HAMPSON, R WALKER	61	700681
ERES	IR		
	BRIDGMAN, P	51	400533
MPP	IR		
	FRANCIS, A	62	301076
REV	IR		
	BETTERIDGE, W RHYS	62	202003
PHAS	IR		
	MENDENHALL, C INGE	07	900143
PHAS	IR		
	HENNING, F WENSEL	33	900128
SPK	IR		
	DEODHAR, G PADALIA	62	300576
SPK	IR		
	MOORE, C	58	601088
SPK	IR		
	ROSENZWEIG, N PORT	60	700901
SPK	IR		
	ROSENZWEIG, N PORT	60	700996
SPK	IR		
	MURAKAWA, K SUWA	52	600942
SPK	IR		
	ALBERTSON, W	38	900122
SPK	IR		
	SEIMENS, W	53	600949
TCON	IR		
	WHITE, G WOODS, S	57	601050
TCON	IR		
	POWELL, R TYE, R	55	601082
THEO	IR		
	ROSENZWEIG, N PORT	60	700996
THEO	IR		
	ROSENZWEIG, N PORT	60	700901
THER	IR		
	DOUGLASS, R HOLDEN	59	700375
THER	IR		
	BARRIAULT, R DREIK	62	300865
THER	IR		
	GOODWIN, T	56	601547
TRT	IR		
	MCCALDIN, J DUWEZ	54	600956
TRT	IR		
	MENDENHALL, C INGE	07	900143
TRT	IR		
	HENNING, F WENSEL	33	900128
VAP	IR		
	MARGRAVE, J	61	700967
VAP	IR		
	HASAPIS, A PANISH	60	700994
VAP	IR		
	DREGER, L	62	300720
VAP	IR		
	DREGER, L	61	300528
VAP	IR		
	DREGER, L MARGRAVE	60	600643
VAP	IR		
	PANISH, M REIF, L	61	700639
VAP	IR		
	HAMPSON, R WALKER	61	700681
VAP	IR		
	PAULE, R	61	601479
CRYS	IR B SYST		
	ARONSON, B STENBER	62	300757
CRYS	IR B SYST		
	ARONSON, B ASELIUS	59	601166
PHAS	IR C		
	NADLER, M KEMPTER	60	300301
REAC	IR CL		
	STEPIN, B CHERNYAK	60	201576
THER	IR O		
	BARRIAULT, R DREIK	62	300865
CPH	IR O 2		
	JAEGER, F	34	900127
CPH	IR O 2		
	WOHLER, L JOCHUM	33	900124
CPH	IR O 2		
	WOHLER, L JOCHUM	33	900124
DH	IR O 2		
	SCHNEIDEREITTI, G	62	301582
DH	IR O 2		
	WOHLER, L WITZMANN	08	900125
DH	IR O 2		
	BILTZ, W	34	900127
DH	IR O 2		
	WOHLER, L JOCHUM	33	900124
DH	IR O 2		
	WOHLER, L JOCHUM	33	900124
VAP	IR O 2		
	CORDFUNKE, E MEYER	62	300572
THER	IR2O 3		
	ALCOCK, C HOOPER	60	601161
VAP	IR O SYST		
	CORDFUNKE, E MEYER	62	301054
MISC	IR O SYST		
	HELVENSTON, E	60	601195
THER	IR O SYST		
	SCHAFER, H JOACHIM	60	601160

K

VAP	KNUDSEN		
	WINTERBOTTOM, W HI	62	300560
VAP	KNUDSEN		
	VETRENKO, E MIKULI	62	300603

L

CTEX	LA		
	ANDRES, K	63	301172
THER	LA		
	MASLOV, P MASLOV	59	601196
BETA	LA		
	BRIDGMAN, P	48	700883
BETA	LA		
	BRIDGMAN, P	48	700884
CPL	LA		
	PARKINSON, D H SIM	51	400557
CPL	LA		
	BERG, J		700760
CPL	LA		
	PARKINSON, D	51	700885
CPL	LA		
	BERMAN, A ZEMANSKY	58	700886
CPL	LA		
	BOORSE, H BERMAN	55	700887

CPL	LA	MONTGOMERY, H PELL	61	700910
CRYS	LA	ZIEGLER, W YOUNG	53	100196
CRYS	LA	HERRMANN, K DAANE	56	700905
CTEX	LA	DASHKOVSKII, A SAV	61	201866
CTEX	LA	BARSON, F LEGVOLD	56	700902
DHT	LA	CAVALLERO, U	43	700895
ERES	LA	ZIEGLER, W YOUNG	53	100196
ERES	LA	COLVIN, R LEGVOLD	60	601389
ERES	LA	ALSTAD, J COLVIN	61	201099
ERES	LA	BRIDGMAN, P	51	400533
ERES	LA	JAMES, N LEGNOLD	62	100206
H	LA	KELLEY, K	60	700891
MPP	LA	SPEDDING, F DAANE	61	700907
PHAS	LA	SPEDDING, F DAANE	57	700872
PMCH	LA	SMITH, J CARLSON	57	700746
REAC	LA	LORIERS, J	49	400542
S	LA	KELLEY, K	60	700891
SPK	LA	MURAKAWA, K	61	300826
SPK	LA	GARSTANG, R	52	100207
SPK	LA	VAN DIJKE BEATTY, S	51	400548
SPK	LA	GRATTON, L	52	400567
SPK	LA	MOORE, C	58	601088
SPK	LA	YATSMIRSKII, K	48	700751
SPK	LA	BURBRIDGE E BURBR	55	601003
SPK	LA	RUBESKA, I	62	600119
SPK	LA	MURAKAWA, K KAMEI	53	601218
SPK	LA	SCHWARZSCHILD, M	57	601047
SPK	LA	MOORE, C	58	700913
THER	LA	PARKINSON, D H SIM	51	400557
VAP	LA	ACKERMANN, R RAUH	62	700840
VAP	LA	BEAVIS, L	60	700878
VAP	LA	ACKERMANN, J RAUH	62	700909
THER	LA +	GREEN, J POLAND, D	60	700882
MPP	LA B	SAMSONOV, G	56	700730
CRYS	LA B 4	FELTEN, E BENDER	58	700857
CEMP	LA B 6	SAMSONOV, G PADERN	59	300143
CEMP	LA B 6	LAFFERTY, J	50	400541
CPH	LA B 6	SAMSONOV, G PADERN	61	700862
CRYS	LA B 6	NESPHOR, V SAMSONO	59	700859
CRYS	LA B 6	ZHDANOV, G ZHURAVL	57	601061
CRYS	LA B 6	MALINCHKOV, O POVI	62	300948
CRYS	LA B 6	SAMSONOV, G GRODSH	56	700733
CRYS	LA B 6	TVOROGOV, N	59	700860
CRYS	LA B 6	BERTAUT, F BLUM, P	52	700870
CTEX	LA B 6	ZHDANOV, G ZHURAVL	57	700731
CTEX	LA B 6	KRIKORIAN, O	60	700847
DH	LA B 6	SAMSONOV, G PADERN	61	700862
MPP	LA B 6	SAMSONOV, G	59	700845
MPP	LA B 6	SAMSONOV, G NESHPO	59	700734
VAP	LA B 6	FESENKO, V BOLGAR	63	301216
MPP	LA B 6	KUDINTSEVA, G POPO	62	301289
COPT	LA B 6	TSAREV, B ILLARION	63	301369
MPP	LA B 6	BLUM, P BERTAUT, F	54	700848
CEMP	LA BORIDE	PADERNO, Y SAMSONO	60	200971
CRYS	LA B SYST	MALYUCHKOV, O POVI	62	300584
PHAS	LA B SYST	JOHNSON, R DAANE	61	201106
REAC	LA C	SCAIFE, D WYLIE, A	58	700863
CEMP	LA C 2	GREENWOOD, N OSBOR	61	201076
CRYS	LA C 2	WARF, J PALENIK, G	60	700849
CRYS	LA C 2	PALENIK, C WARF, J	62	700850
CRYS	LA C 2	BREDIG, M	60	700852
CRYS	LA C 2	SPEDDING, F GSCHNE	58	700858
CRYS	LA C 2	ATOJI M	61	700864
CRYS	LA C 2	ATOJI, M MEDRUD, R	59	700867
CRYS	LA C 2	ATOJI, M GSCHNEIDE	58	700868
CTEX	LA C 2	KRIKORIAN, O	60	700847
REAC	LA C 2	KOVALCHENKO, M NES	58	700869
SPK	LA C 2	LOWRIE, R	60	701014
SPK	LA C 2	LOWRIE, R	61	700956
SPK	LA C 2	LOWRIE, R	61	700736
THER	LA C 2	CHUPKA, W BERKOWIT	58	700866
CRYS	LA C 3	ATOJI, M WILLIAMS	60	700861
VAP	LA CL3	NOVIKOV, G BAEV, A	62	300686
CEMP	LA2C 3	GREENWOOD, N OSBOR	61	201076
PHAS	LA C SYST	ANON	55	601265
PHAS	LA C SYST	WARF, J PALENIK, G	60	600636
PHAS	LA C SYST	SPEDDING, F GSCHNE	61	700687
PHAS	LA C SYST	SPEDDING, F GSCANE	59	700853

CRYS	LA N	YOUNG, R ZIEGLER	52	100205
CRYS	LA N	YOUNG, R ZIEGLER	52	700856
CRYS	LA N	KLEMM, W WINKELMAN	56	700874
MPP	LA N	LYUTAYA, M SAMSONO	63	301529
THER	LA N	KELLEY, K	37	700865
THER	LA N	BAUGHAN, E	59	700876
CRYS	LA N SYST	IANDELLI, A	37	601276
DHD	LA O	CHUPKA, W INGHRAM	56	700925
DHD	LA O	GOLDSTEIN, H	61	201216
DHD	LA O	WALSH, P WHITE, D	58	700806
DHD	LA O	WALSH, P GOLDSTEIN	60	700924
F	LA O	BREWER, L CHANDRAS	59	700892
H	LA O	KELLEY, K	60	700891
PHAS	LA O	FOEX, M	61	201153
S	LA O	KELLEY, K	60	700891
SPK	LA O	AKERLIND, L	62	300610
SPK	LA O	MURTHY, N	61	301087
SPK	LA O	HATUECLER, S ROSEN	59	700759
SPK	LA O	ROSEN, B	51	700890
SPK	LA O	AKERLIND, L	62	700894
THER	LA O	BREWER, L	53	700921
VAP	LA O	GOLDSTEIN, H WALSH	61	700889
VAP	LA O	GOLDSTEIN, H WALSH	60	700896
VAP	LA O	KULVARSHAYA, B MAS	60	301064
VAP	LA O	WALSH, P GOLDSTEIN	60	700924
CPH	LA2O 3	GOLDSTEIN, H NGILS	59	601198
CPH	LA2O 3	BLOMEKE, J O ZIEGL	51	400562
CPL	LA2O 3	JUSTICE, B WESTRUM	63	300906
CPL	LA2O 3	GOLDSTEIN, H	58	601551
CPL	LA2O 3	GOLDSTEIN, H NEILS	59	700836
CRYS	LA2O 3	KOEHLER, W WOLLAN	53	700754
CRYS	LA2O 3	JOHNSON, Q TEMPLET	61	700881
CRYS	LA2O 3	IANDELLI, A	56	700897
DF	LA2O 3	COUGHLIN, J	54	700914
DH	LA2O 3	HUBER, E HOLLEY, C	53	700900
DH	LA2O 3	COUGHLIN, J	54	700914
DH	LA2O 3	WARTENBERG, H	59	700923
DHD	LA2O 3	WALSH, P GOLDSTEIN	60	700924
H	LA2O 3	BLOMEKE, J O ZIEGL	61	400562
MPP	LA2O 3	TRESVYATSKIY, S CH	61	300440
MPP	LA2O 3	NAGASAWA, S	50	400530
PHAS	LA2O 3	SCHNEIDER, S ROTH	60	700747
PHAS	LA2O 3	EYRING, L VORRES	60	700748
PHAS	LA2O 3	LAMBERTSON, W GUNZ	52	700762
PHAS	LA2O 3	WOLF, L SCHWAB, H	61	201408
REAC	LA2O 3	KELER, E GODINA, N	61	300387
REAC	LA2O 3	MOROZOV, I KORSHUN	58	700753
TRT	LA2O 3	LAMBERTSON, W GUNZ	52	700762
S	LA2O 3	BLOMEKE, J O ZIEGL	51	400562
S	LA2O 3	KELLEY, K KING, E	61	700915
THER	LA2O 3	KING, E WELLER, W	61	300712
THER	LA2O 3	INGHRAM, M CHUPKA	57	601067
THER	LA2O 3	BLOMEKE, J O ZIEGL	51	400562
THER	LA2O 3	BREWER, L	53	700906
VAP	LA2O 3	TOSIM, S	57	601505
VAP	LA2O 3	GOLDSTEIN, H	61	201216
VAP	LA2O 3	WALSH, P WHITE, D	58	700806
VAP	LA2O 3	WALSH, P GOLDSTEIN	60	700888
VAP	LA2O 3	GOLDSTEIN, H WALSH	61	700889
VAP	LA2O 3	ACKERMAN, J THORN	61	700908
VAP	LA2O 3	GOLDSTEIN, H	60	201018
VAP	LA2O 3	WALSH, P GOLDSTEIN	60	700924
DH	LA O SYST	WALSH, P N DEVER	61	700642
MISC	LA O SYST	LORIERS, J	49	400542
PHAS	LA SI O SYST	TOROPOV, N BONDAR	60	201506
DH	LANTHANIDE IONS	YATSIMIRSKII, K B	49	400583
THER	LANTHANIDE IONS	YATSIMIRSKII, K B	49	400583
THEO	LANTHANIDES	SCHENK, P	49	400579
VAP	LANTHANIDES	ZADUMKIN, S TAMBIE	61	301020
ELCH	LATTICE STRUCTURE	BETHE, H	63	301131
PHAS	LA U O SYST	HILL, D	62	201873
MPP	LIGHT	PLYLER, E BLAINE	55	600720
DH	LI2O	BERKOWITZ, J CHUPK	59	700892
MSP	LI2O	BERKOWITZ, J CHUPK	59	700892
THER	LI2O	BERKOWITZ, J CHUPK	59	700892
VAP	LI2O	FIRSOVA, L NESEMEY	60	200761
MPP	LIQUID METALS	SAMARIN, A	60	400595
CPH	LIQUIDS	AFENKOV, N	62	301392

MPP	LIQUIDS	GROSSE, A	61	301463
THEO	LIQUIDS	EDWARDS, S	62	301438
THEO	LIQUIDS	GROSSE, A KIRSHENB	62	301143
THEO	LIQUIDS	GORDON, R	61	202041
THEO	LIQUIDS	GROSSE, A	63	202043
THEO	LIQUIDS	HIRSCHFELDER, J CU	54	202051
THEO	LIQUIDS	GRIGOROVICH, V	60	301233
THEO	LIQUIDS	GROSSE, A KIRSHENB	63	301236
THEO	LIQUIDS	PREDVODITELEV, A	63	301322
CPH	LIQUIDS	KUDRYAYTSEV, B	62	300363
CPL	LU	JENNINGS, L MILLER	60	201049
DH	LU	WHITE, D	61	201217
VAP	LU	WHITE, D WALSH, P	61	301014
VAP	LU	WHITE, D WALSH, P	60	301622
PHAS	LU B 2	PRZYLYLSKA, M REDD	63	300962
CEMP	LU B 6	SAMSONOV, G PADERN	59	300143
VAP	LU O	KULVARSHAYA, B MAS	60	301064

M

CRYS	M O	DUAN, F NAY BEN, M	63	301213
VAP	MASS SPEC	HILL, H REED, R	63	301243
MPP	MATERIALS	STEWARD, R JOHNSON	61	301598
PHAS	MATERIALS	LOVEJOY, D	63	202087
REV	MATERIALS	KORNILOV, I POLYAK	63	202080
REV	MATERIALS	HAUCK, J	63	202048
REV	MATERIALS	BARTLETT, E	63	201997
THEO	MELTING	ARDELL, A	63	301174
THEO	MELTING	BABB, S	63	301177
THEO	MELTING	ROTT, L	62	301331
DF	METAL BORIDES	LANGER, S	61	700939
PHAS	METAL BORIDES	LANGER, S	61	700939
THER	METAL BORIDES	LANGER, S	61	700939
VAP	METAL BORIDES	LANGER, S	61	700939
DF	METAL CARBIDES	LANGER, S	61	700939
PHAS	METAL CARBIDES	LANGER, S	61	700939
THER	METAL CARBIDES	LANGER, S	61	700939
VAP	METAL CARBIDES	LANGER, S	61	700939
SPK	METAL COMPOUND	KLIMOV, V	61	700670
CEMP	METAL OXIDES	OREILLY, D	61	700633
DF	METAL OXIDES	GLEISER, M	61	700616
REV	METAL OXIDES	GLEISER, M	61	700616
E	METALLIC COMPOUND	SAMSONOV, G SHULIS	62	300756
BOOK	METALLURGY	VULF, B ROMADIN	62	301614
BOOK	METALLURGY	HUME-ROTHERY, W	62	202059
VAP	METALS	LYUBITOV, YU	59	301295
BETA	METALS	MITRA, S JOSHI, S	61	700630
CPH	METALS	LOWENTHAL, G	63	300936
CPH	METALS	PCHELKIN, I	61	300649
CPL	METALS	ELIASHBERG, G	62	300881
CPL	METALS	NITRA, S JOSHI, S	61	700630
CRYS	METALS	SMALLMAN, R	63	301157
CTEX	METALS	HANAK, J DAANE, A	61	201378
DHD	METALS	SHULISHOVA, O	62	301587
DHT	METALS	MORIN, F MAITA, J	63	301043
E	METALS	LADD, M LEE, W	62	300575
MISC	METALS	MCCULLOUGH, R	62	301761
MPP	METALS	OSMININ, Y	62	301152
MPP	METALS	EREMENKO, V NIZHEN	61	300537
MPP	METALS	TIMOFEEVICHEVA, O	61	300540
MPP	METALS	MCQUEEN, R MARSH	60	200777
MPP	METALS	CHAUDRON, G	61	700557
MPP	METALS	GARBER, R GINDIN	61	700673
MSP	METALS	VELISEK, J	63	202152
THEO	METALS	LIBBY, W	62	202086
REV	METALS	COOPER, T SRP, O	63	202019
THEO	METALS	ENIG, J	63	202030
THEO	METALS	BREWER, L	63	202009
VAP	METALS	BURTSEV, V SAMARIN	62	202012
PHAS	METALS	TSAREV, B KUDINTSE	58	301161
PHAS	METALS	NORTON, J OGILVIE	57	201086
REAC	METALS	MARKSTEM, H	63	301532
REAC	METALS	WILSON, B	60	200896
REV	METALS	SPEDDING, F DAANE	60	200853
REV	METALS	STADELMAIER, H	61	201365
REV	METALS	PECKNER, D	62	201944
REV	METALS	VAN ARKEL, A	62	201987
SURF	METALS	PUGACHEVICH, P LAZ	60	200878

SURF	METALS	STRAUSS, S	60	201065
SURF	METALS	MONMA, K	60	201440
TCON	METALS	POWELL, R BLANPIED	54	600906
TCON	METALS	LEBEDEV, V	60	200842
TCON	METALS	MENDELSSOHN, K ROS	61	201403
TCON	METALS	EWING, C WALKER, B	62	201768
theo	METALS	KAUFMAN, L CLOUGHE	63	h 301495
THEO	METALS	HARRISON, W	63	301468
THEO	METALS	SAMOILOV, O	61	300539
THER	METALS	ESIN, O SRYVALIN	60	300276
THER	METALS	WHITE, J	60	300318
THER	METALS	EDELEANU, C LITTLE	60	200838
TRT	METALS	STRAUSS, S	60	201065
TRT	METALS	GOPAL, R MOHD	62	301461
VAP	METALS, ALKALI	SHPILRAYN, E ASINO	62	301099
CPH	METALS, LIQUID	SOLTYK, V	62	301158
REV	METALS, LIQUID	FROST, B	62	301451
THER	METALS, LIQUID	KIM, W	62	301499
CPH	MG	WILLIAMS, N N	61	700659
CPL	MG	COLLINS, M	62	300870
CPL	MG	MARTIN, D	61	300666
	MG	LAWLEY, A	60	200801
CRYS	MG	GETTE, E FOOTE, F	36	700510
CTEX	MG	BESSERER, C	58	700929
DH	MG	GOLDSMITH, A HIRSC	60	700930
ERES	MG	BRIDGMAN, P	51	400533
MPP	MG	BESSERER, C	58	700929
PHAS	MG	GOLDSMITH, A HIRSC	60	700930
PHAS	MG	BEREZHNOI, A KORDY	62	201563
REAC	MG	EVSTYUKHIN, A	59	200852
RHO	MG	MCGONIGAL, P KIRSH	62	201532
SPK	MG	CRISP, R WILLIAMS	60	201000
SPK	MG	PENKIN, N SHABANOV	62	601601
SPK	MG	CODLING, K	61	600775
TCON	MG	BESSERER, C	58	700929
THER	MG	BARRIAULT, R DREIK	62	300865
THER	MG	DEWING, E	60	201204
THER	MG	WILLIAMS, N N	61	700659
VAP	MG	FUJINO, S OKADA, M	62	301452
VAP	MG	GOLDSMITH, A HIRSC	60	700930
VAP	MG	HANLIN, H	60	700951
VAP	MG	FRANZEN, J HINTENB	61	700970
VAP	MG	GRJOTHEIM, K HERST	61	200990
REAC	MG B	MARKOUSKII, L KAPU	62	201722
CRYS	MG B 2	JONES, M MARSH, R	54	300909
CRYS	MG B 2	RUSSELL, V HIRST	53	300968
REAC	MG B 6	MARKOVSKII, L	62	301530
REAC	MG B12	MARKOVSKII, L	62	301530
PHAS	MG BORIDES	CHRETIEN, A DUHART	62	300536
PHAS	MG B SYST	DUHART, P	62	300875
PHAS	MG B SYST	MARKOVSKII, L KOND	55	300942
PHAS	MG B SYST	MARKOVSKII, L KOND	55	300943
CRYS	MG CE SYST	BELETSKII, M GALPE	61	200827
CRYS	MG IR SYST	FERRO, R RAMBALDI	62	201626
VAP	MG N	SMITH, J	62	201743
KIN	MG3N 2	DERRAS, R PAIBASSI	62	201918
THER	MG3N 2	SCHICK, H ANTHROP	63	301579
CRYS	MG ND SYST	BELETSKII, M GALPE	61	200827
CPH	MG O	VICTOR, A DOUGLAS	60	700949
CPH	MG O	FIELDHOUSE, I LANG	60	601583
CPL	MG O	VICTOR, A DOUGLAS,	60	700949
REAC	MG O	KOMAREK, K COUCOUL	63	301269
REAC	MG O	RYABCHIKOV, I MIKU	62	301336
REAC	MG O	RYABCHIKOV, I MIKU	63	301337
TRT	MG O	SCHNEIDER, S	63	301348
CPH	MG O	VICTOR, A DOUGLAS	63	301372
CPL	MG O	LIEN, W	62	201454
CRYS	MG O	COCCO, A SCHROMEK	61	201211
CTEX	MG O	FIELDHOUSE, I LANG	60	601583
ERES	MG O	MITOFF	62	201674
H	MG O	VICTOR, A DOUGLAS	60	700949
MISC	MG O	LADD, M LEE, W	60	201322
MPP	MG O	WUENSCH, B VASILOS	62	201836
MPP	MG O	WUENSCH, B VASILOS	61	301018
MPP	MG O	GANESAN, S	62	201559
PHAS	MG O	HINZ, I DIETZEL, A	62	301472
PHAS	MG O	MASSAZZA, F	61	201293
REAC	MG O	LEONOV, A	61	301522

REAC	MG O	TOGURI, J	60	201009
REAC	MG O	GRJOTHEIM, K HERST	61	200990
REAC	MG O	POLUNINA, G KOVBA	61	201624
REAC	MG O	SOLACOLU, S	61	201694
SPK	MG O	NICHOLLS, R	62	601625
SPK	MG O	NAZIMOVA, N	60	201227
SPK	MG O	ORTENBERG, F	61	300821
SPK	MG O	PESIC, D	60	701002
SPK	MG O	ORTENBERG, F	61	300795
SPK	MG O	BREWER, L TRAJMA	62	201780
SPK	MG O	BREWER, L TROJMAR	62	300788
SPK	MG O	PESIC, D	60	600656
SPK	MG O	VEITS, I GURVICH	57	600899
SPK	MG O	LAGERQVIST, A UHLE	49	600923
SPK	MG O	LAGERQVIST, A UHLE	49	600924
SPK	MG O	TRAJMAR, S	61	700962
SPK	MG O	NAZIMOVA, N SOKOLO	61	700671
SPK	MG O	SOLOKOV, V NEZIMOV	60	201622
TCON	MG O	FIELDHOUSE, I LANG	60	601583
TCON	MG O	ADAMS, M	54	600961
THEO	MG O	TAWDE, N SREEDHARA	62	300782
THER	MG O	SCHICK, H ANTHROP	62	300995
TRT	MG O	MCNALLY, R PETERS	61	600828
VAP	MG O	METSON, G	63	301536
VAP	MG O	ALTMAN, R	63	300844
VAP	MG O	GILBREATH, J	55	601274
CPH	MG O	VICTOR, A DOUGLAS	60	202163
CEMP	MG OXIDES	PALGUEV, S NECEIMI	62	201717
DHD	MG OXIDES	VEITS, I GURVICH	56	700964
THER	MG OXIDES	DEWING, E	60	201204
THER	MG OXIDES	VEITS, I GURVICH	56	700964
CEMP	MISC	KISER, R	60	200784
CPH	MISC	NAGASAKI, S TAKAGI	48	400598
CPL	MISC	BARBER, S MARTIN	59	600650
DH	MISC	BARANOVSKY, V	62	300366
DF	MISC	ANON	60	300226
ELCH	MISC	STERN, K		300305
EMF	MISC	GERASIMOV, V GROMO	61	300445
MPP	MISC	SMIRNOVA, V ORMONT	59	300267
MPP	MISC	WICHERS, E	62	300359
MPP	MISC	KIRILLIN, V VUKALO	61	300378
MPP	MISC	GOLDANSKIY, V KAGA	60	400589
MPP	MISC	TRETYACHENKO, G KR	61	400610
MSP	MISC	JENCKLE, L	61	300322
MSP	MISC	BRYUKAHNOV, A GOLU	62	400614
MSP	MISC	ALEKSEYEVSKIY, N	58	400600
PHAS	MISC	TISZA, L	61	700592
PMCH	MISC	EVERHART, J LINDLI	43	600907
SPK	MISC	HERTZBERG, G	59	200785
SPK	MISC	MAJUMDAR, K VARSHN	54	600886
SPK	MISC	MAJUMDAR, K VARSHN	54	600887
SPK	MISC	MAJUMDAR, K VARSHN	54	600888
SPK	MISC	MAJUMDAR, K VARSHN	54	600889
SPK	MISC	VARSHNI, Y MAJUMDA	56	600895
SPK	MISC	FERRARO, J R	61	700571
THEO	MISC	MASLOV, P MASLOV	61	700538
THEO	MISC	KLIUCHNIKOV, N	60	300747
THEO	MISC	AFANASYEV, A	61	400603
THEO	MISC	BADYLKES, I	61	700593
THEO	MISC	KAROPETYANTS, M	61	700617
THER	MISC	ANON	60	300226
THER	MISC	HECHT, C	62	300365
THER	MISC	TISZA L	61	700592
VAP	MISC	KOML[illegible], G VETRENKO	58	300421
ZKP	MISC	BAIBUZ, V	62	300601
CRYS	MN	KRYISYAKEVICH, P	60	600698
DH	MN	GOLDSMITH, A HIRSC	60	700930
ERES	MN	NOVIKOV, A TYSPIN	59	201632
PHAS	MN	TOPCHIASHVILI, L	60	201238
PHAS	MN	GOLDSMITH, A HIRSC	60	700930
SPK	MN	GOODMAN, NOLDEKE	62	300789
SPK	MN	ROSENZWEIG, N PORT	60	700901
SPK	MN	ROSENZWEIG, N PORT	60	700996
SPK	MN	MURAKAWA, K KAMEI	53	601218
THEO	MN	ROSENZWEIG, N PORT	60	700996
THEO	MN	ROSENZWEIG, N PORT	60	700901
THER	MN	SCHICK, H ANTHROP	62	300995
THER	MN	BUTLER, J F MCCABE	61	700629

VAP	MN	GOLDSMITH, A HIRSC	60	700930
VAP	MN	HANLIN, H	60	700951
VAP	MN	BUTLER, J F MCCABE	61	700629
REAC	MN B	MARKOVSKII, L	62	301530
CRYS	MN B 2	ARONSSON, B	60	201380
CRYS	MN B 2	BINDER, I POST, B	60	200779
REAC	MN B 2	MARKOVSKII, L	62	301530
MPP	MN B 4	FRUCHART, R MICHEL	60	300241
PHAS	MN B P SYST	RUNDQVIST, S	62	300546
CPL	MN BR2	STOUT, J	58	201122
REAC	MN2B	MARKOVSKII, L	62	301530
REAC	MN3B 4	MARKOVSKII, L	62	301530
ELCH	MN BORIDES	ALENARD, S	61	201402
CEMP	MN B SYST	CADEVILLE, M MEYER	62	202013
CRYS	MN5C 2	SENATEUR, J FRUCHA	62	201957
THER	MN7C 3	GOKCEN, N FUJISHIR	63	301456
THER	MN7C 3	ANON	60	700992
THER	MN7C 3	BUTLER, J F MCCABE	61	700629
THER	MN7C 3	ANON	60	700904
VAP	MN7C 3	ANON	60	700904
VAP	MN7C 3	ANON	60	700992
VAP	MN7C 3	ANON	60	600666
VAP	MN7C 3	BUTLER, J F MCCABE	61	700629
DF	MN23C6	ALEXEEV, V SCHWARZ	61	300405
TCON	MN F 2	SLACK, G	61	201125
DH	MN N SYST	SHCHUKAREV, S MORO	61	700666
PHAS	MN N SYST	LIHL, F ETTMAYER	62	301025
THER	MN N SYST	AGLADZE, R I MANPO	61	700551
REAC	MN N SYST	AGLADZE, R I MANP	61	700551
CRYS	MN O	HOCH, M	63	301477
CRYS	MN O	BIRCHENALL, C	60	200775
DHD	MN O	HULDT, L LAGERQVIS	52	600764
PHAS	MN O	BREWER, L	49	601633
PHAS	MN O	GATTOW, G	62	201758
SPK	MN O	LOH, E NEWMAN, R	61	700528
SPK	MN O	JOSHI, K	62	201984
THER	MN O	SCHICK, H ANTHROP	62	300995
CEMP	MN O 2	SRB, V	61	201088
CRYS	MN O 2	VEDAM, K	61	700961
CRYS	MN O 2	KONDRASHEV, Y	61	700942
MPP	MN O 2	SRB, V	61	201083
MPP	MN O 2	GATTOW, G GLEMSER	61	700576
PHAS	MN O 2	KONDRASHEV, Y	61	700942
PHAS	MN O 2	GATTOW, G GLEMSER	61	700576
PHAS	MN O 2	FISHBURN, H PILL	61	201360
PHAS	MN O 2	BHIDE, V DAMLE, R	61	201596
REAC	MN O 2	GATTOW, G GLEMSER,	61	700576
TRT	MN O 2	GATTOW, G GLEMSER	61	700576
CRYS	MN3O 4	SATOMA, K	61	201025
REAC	MN OXIDES	ANIKEEV, V LYUBAN	60	201035
DHD	MN OXIDES	ANIKEEV, V LYUBAN	60	201035
VAP	MN OXIDES	GLEMSER, O WEIZENK	61	201441
THER	MN OXIDES	BLUMENTHAL, R WHIT	61	600829
ELCH	MN OXIDES	BLUMENTHAL, R WHIT	61	600829
ERES	MN O SYST	BHIDE, V DANI, R	61	201324
MPP	MN O SYST	GATTOW, G GLEMSER	61	700577
PHAS	MN O SYST	KLINGSBERG, C RUST	60	700518
REAC	MN O SYST	GATTOW, G GLEMSER	61	700577
PHAS	MN RE SYST	SAVITSKII, E TYLKI	61	700625
THER	MN SI SYST	GOLUTVIN, KOZLON	63	301228
PHAS	MN SI B SYST	ARONSSON, B ENGSTR	60	201348
PHAS	MN SI O SYST	SINGLETON, E CARPE	62	201560
PHAS	MN TA SYST	SAVITSKII, E KAPET	60	201701
PHAS	MN TI SYST	SAVITSKII, E KOPET	60	201261
PHAS	MN TI ZR O SYST	WYDER, W HOCH, M	62	300548
DH	MN W O SYST	PROSHINA, Z	60	201249
PHAS	MN ZR SYST	SAVITSKII, E KOPET	60	201261
BETA	MO	KRUPNIKOU, K BAKAN	63	301149
BIB	MO	WENSRICH, C	60	700972
BIB	MO	WOHLL, M	60	700723
BIB	MO	RICHERT, E BECKETT	49	700564
CEMP	MO	COMSA, G GELBERG	61	700940
COPT	MO	COFFMAN, J COULSON	61	701040
CPH	MO	JOHNSON, R	60	301488
CPH	MO	RASOR, N MCCLELLAN	60	700984
CPH	MO	KIRILLIN, V SHEIND	61	300921
CPH	MO	RUDKIN, R	60	700898
CPH	MO	FINCH, R	61	700547

CPH	MO	KIRILLIN, V SHEIND	62	300734
CPH	MO	RASOR, N MCCLELLAN	60	700896
CPH	MO	CHEKHOVSKOI, V	62	300633
CPH	MO	LEHMAN, G	60	300304
CPH	MO	KIRILLIN, V SHEIND	61	300332
CPH	MO	KARAREYA, L	61	300344
CPH	MO	KIRILLIN, V SHEIND	61	300426
CPH	MO	KIRILLIN, V SHEIND	62	601564
CPH	MO	TAYLOR, R	61	201250
CPH	MO	BRONSON, H CHISHOL	33	700561
CPH	MO	LAZAREVA, L KANTOR	61	700631
CPL	MO	FINCH, R	61	700547
CPL	MO	CHEKHOVSKOI, V	62	300633
CPL	MO	BORELIUS, G	60	601168
CPL	MO	TAYLOR, R	61	201250
CPL	MO	CLARK, C	62	601563
CPL	MO	FEATHERSTON, F NEI	63	301444
CPL	MO	BRYANT, C KEESOM	61	600831
CPL	MO	SHARAN, B	61	301070
CRYS	MO	COFFMAN, J COULSON	61	701040
CRYS	MO	EDWARDS, J SPEISER	51	601179
CRYS	MO	GETTE, E FOOTE, F	35	700510
CRYS	MO	LU, S CHANG, Y	41	700512
CRYS	MO	AGGARWAL, P GOSWAM	57	700514
CRYS	MO	MATYUSHENKO, N	62	301150
CTEX	MO	RASOR, N MCCLELLAN	60	700984
CTEX	MO	EDWARDS, J SPEISER	51	601179
CTEX	MO	BESSERER, C	58	700929
CTEX	MO	NOWOTNY, H LAUBE	61	600844
DH	MO	KIRILLIN, V SHEIND	62	601564
DF	MO	COFFMAN, J COULSON	61	701040
ERES	MO	TAYLOR, R	61	201250
ERES	MO	TYE, R	61	201117
ERES	MO	RUDKIN, R	60	700898
ERES	MO	FINCH, R	61	700547
ERES	MO	BRIDGMAN, P	51	400533
ERES	MO	MARGOTIN, P DURAND	62	201863
H	MO	KIRILLIN, V SHEIND	61	300921
MISC	MO	HAMPEL, C	61	200889
MPP	MO	HOUCK, J	61	701003
MPP	MO	RASOR, N MCCLELLAN	60	700896
MPP	MO	KOPETSKIY, CH.	62	301270
MPP	MO	MING, N FAN, T LI	63	301304
MPP	MO	BESSERER, C	58	700929
MPP	MO	ARGENT, B MILNE, G	60	201039
MPP	MO	RICHERT, E BECKETT	49	700564
MPP	MO	BADIALI, M KIRSHEN	63	301404
PHAS	MO	COFFMAN, J COULSON	61	701040
PHAS	MO	SHAFFER, P	61	700941
PHAS	MO	BRILLIANTOV, N STA	61	300807
PHAS	MO	BRILLIANTOV, N STA	61	300807
PHAS	MO	HAWORTH, C	60	201017
PHAS	MO	FUNKE, V NOVIKOVA	62	201704
REAC	MO	FRANTSEVICH, I LAV	59	200869
REAC	MO	KOMAR, A TALANIN	60	200843
REAC	MO	DEUTSCH, N ERVIN	60	500123
REAC	MO	KUBASCHEWSKI, O HO	60	201038
REAC	MO	EREMENKO, V VELIKA	59	201279
REAC	MO	ENGELKE, J HALDEN	60	201529
REAC	MO	VEROT, J FORESTIER	61	201528
REAC	MO	ZELIKMAN, A KREIN	62	201861
REAC	MO	ANDREEVA, V ALEKSE	62	201814
REV	MO	SYRE, R	61	201579
REV	MO	WOHLL M	60	701053
REV	MO	RICHERT, E BECKETT	49	700564
SPK	MO	ALLEN, R GLASIER	60	200828
SPK	MO	ROGOSA, G SCHWARZ	53	500124
SPK	MO	SHADMI, Y	61	700954
SPK	MO	CLAUS, H ULMER, K	63	202017
SPK	MO	TREES, R	61	701067
SPK	MO	ROSENZWEIG N PORT	60	700996
SPK	MO	SWEENEY, W SEAL, R	61	201112
SURF	MO	RUDKIN, R	60	700898
TCON	MO	RUDKIN, R	60	201901
TCON	MO	BESSERER, C	58	700929
TCON	MO	RASOR, N MCCLELLAN	60	700896
TCON	MO	RASOR, N MCCLELLAN	60	700984
TCON	MO	TYE, R	61	201117

TCON	MO	LEBEDEV, V	61	201312
THEO	MO	ROSENZWEIG, N PORT	60	700996
THER	MO	RASOR, N MCCLELLAN	60	200960
VAP	MO	BABELIOWSKY, T	62	300858
VAP	MO	CANO, G	62	301423
VAP	MO	COFFMAN, J COULSON	61	701040
VAP	MO	GLEMSER, O HAESELE	62	201927
PHAS	MO AL C	JEITSCHKO, W NOWOT	63	301486
H	MO B	MEZAKI, R TILLEUX	62	601617
S	MO B	MEZAKI, R TILLEUX	62	601617
H	MO B 2	MEZAKI, R TILLEUX	62	601617
PHAS	MO B 2	FORELIK, C YELYUTI	62	300884
S	MO B 2	MEZAKI, R TILLEUX	62	601617
CRYS	MO B 2	GORELIK, C ELYUTIN	62	301230
DH	MO B 4	SHCHUKAREV, S VASI	61	201413
PHAS	MO B 4	CHRETIEN, A HELGOR	61	201084
H	MO2B	MEZAKI, R TILLEUX	62	601617
S	MO2B	MEZAKI, R TILLEUX	62	601617
MPP	MO2B 5	MALYUCHKOV, O POVI	62	202095
EMF	MO BORIDES	BECK, W	61	300477
REAC	MO B SYST	SAMSONOV, G STRASH	62	300990
CEMP	MO C	INGOLD, J	63	301251
CRYS	MO C	CLOUGHERTY, E LOTH	61	600843
CRYS	MO C	KOVALSKII, A SEMEN	59	201671
CRYS	MO C	KAYE, G	62	201909
PHAS	MO C	CLOUGHERTY, E LOTH	61	600843
PHAS	MO C	NADLER, M KEMPTER	60	300301
CPH	MO2C	NEEL, D PEARS, C	61	300146
CRYS	MO2C	FRIES, R KEMPTER	60	701000
CRYS	MO2C	PARTHE, E	62	601630
DF	MO2C	GLEISER, M CHIPMAN	62	301053
PHAS	MO2C	NADLER, M KEMPTER	60	700903
THER	MO2C	SCHICK, H ANTHROP	63	301580
THER	MO3C 2	SCHICK, H ANTHROP	63	301580
DF	MO C SYST	GLEISER, M CHIPMAN	62	300607
THER	MO C SYST	CUNNINGHAM, G WARD	63	301208
DF	MO C SYST	ALEKSEEV, V SHVART	62	300846
REAC	MO C SYST	SAMSONOV, G STRASH	62	300990
THER	. MO C SYST	ALEKSEEV, V SHVART	62	300846
THER	MÔ CARBONYLS	KAWAI, K MURATA, H	60	200805
REAC	MO CE	GAVMEMAHN, F BLANC	62	201520
SPK	MO CL5	BADER, R	61	201260
DH	MO F 6	SETTLE, J FEDER, H	61	300740
SPK	MO F 6	CLAASSEN, H SELIG	62	201854
PHAS	MO HF SYST	TAYLOR, A	61	201207
THER	MO HALIDES	SHCHUKAREV, S VASI	61	201459
THER	MOLECULES	SEIGEL, B SEIGEL	63	301361
SPK	MONATOMIC GASES	JUDD, B	62	300804
THER	MONATOMIC GASES	GORDON, J	61	300639
THER	MONATOMIC GASES	POLAND, D GREEN, J	62	300758
THER	MONATOMIC GASES	GURVICH, L KVLIVDZ	61	300457
THER	MONATOMIC GASES	GURVICH, I KVLIVID	62	400602
S	MONATOMIC IONS	VDOVENKO, U SUGLOB	58	601155
CRYS	MO N	TROITSKAMA, N PINS	63	202147
CRYS	MO N	TROITSKAYA, N PINS	59	200858
MPP	MO N	SAMSONOV, G VERKHO	62	300997
CEMP	MO NITRIDES	SAMSONOV, G	60	700947
DH	MO NITRIDES	SAMSONOV, G	60	700947
REV	MO NITRIDES	SAMSONOV, G	60	700947
PHAS	MO N SYST	TROITSKAYA, N V PI	61	700601
CRYS	MO O	MAGNELI, A	60	600617
MSP	MO O	DEMAUA, G BURNS, R	60	601163
CRYS	MO O 2	CHANEY, W	61	701068
THER	MO O 2	RAPP, R	63	301326
DF	MO O 2	GLEISER, M CHIPMAN	62	301053
DH	MO O 2	KRESTOVNIKOV, A	62	300930
MSP	MO O 2	DEMAUA, G BURNS, R	60	601163
REAC	MO O 2	KOZMANOV, Y	60	201005
VAP	MO O 2	PLANTE, E R	60	300141
CRYS	MO O 3	CHANEY, W	61	701068
CRYS	MO O 3	YODA, E	60	600855
DF	MO O 3	GLEISER, M CHIPMAN	62	300607
DF	MO O 3	ACKERMANN, A THORN	60	601174
DH	MO O 3	KRESTOVNIKOV, A	62	300930
KIN	MO O 3	VASILEV, K STOICHK	58	200995
MSP	MO O 3	DEMAUA, G BURNS, R	60	601163
REAC	MO O 3	FUNAKI, K TADAHARU	50	500117
REAC	MO O 3	VASILEV K STOICHK	58	200995

VAP	MO O 3	HOERBE, R KNACKE	61	300461
VAP	MO O 3	GULBRANSEN, E	63	300891
VAP	MO O 3	SPITSYN, V ZIMAKOV	61	301593
REAC	MO3O	KIHLBORG, L	62	202068
PHAS	MO OXIDE	KIHLBORG, L	59	201174
CPH	MO OXIDES	KING, E WELLER, W	60	700973
CPL	MO OXIDES	KING, E WELLER, W	60	700973
CRYS	MO OXIDES	OZEROV, R	55	701064
DHT	MO OXIDES	KING, E WELLER, W	60	700973
PHAS	MO OXIDES	KING, E WELLER, W	60	700973
S	MO OXIDES	KING, E WELLER, W	60	700973
THER	MO OXIDES	KING, E WELLER, W	60	700973
PHAS	MO O SYST	RODE, E LYSANOVA	62	201843
CRYS	MO O SYST	KIHLBORG, L	63	301498
KIN	MO O SYST	GULBRANSEN, E	63	301465
PHAS	MO O SYST	ANON	60	701015
VAP	MO O SYST	ANON	60	701015
REAC	MO O C SYST	HEGEDUS, A NEUGEBR	60	200789
PHAS	MO OS	TAYLOR, A DOYLE, N	62	301026
PHAS	MO RE SYST	FENG, C LEVESQUE	61	300530
PHAS	MO RH SYST	ANDERSON, E HUME-R	60	200969
PHAS	MO RU SYST	ANDERSON, E HUME R	60	201071
ERES	MO SI2	NESHPOR, V SAMSONO	62	301037
THER	MO SI2	BOLGAR, A	61	700938
VAP	MO SI2	BOLGAR, A	61	700938
ERES	MO3SI	NESHPOR, V SAMSONO	62	301037
ERES	MO5SI3	NESHPOR, V SAMSONO	62	301037
VAP	MO SI SYST	HASAPIS, A MELVEGE	61	701039
PHAS	MO TI ZR SYST	HOCH, M DESJARDIN	62	300899
PHAS	MO V SYST	KORNILOV, I POLYAK	61	201242
PHAS	MO V C SYST	RUDY, E RUDY, E	62	900222
DHT	MO X2	SHUKUROV, T NIKOLS	61	201907
DHT	MO X3	SHUKUROV, T NIKOLS	61	201907
PHAS	MO ZR C SYST	WALLACE, T GUTIERR	63	301375

N

CEMP	N	SAMSONOV, G NESHPO	59	201052
SPK	N	BAER, P MIESCHER	52	600729
SPK	N	PILCHER, G SKINNER	62	301044
THER	N	GERSH, S	47	900216
CPH	N 2	WILLIAMS, N N	61	700659
DH	N 2	GLOEKLER	61	300636
DHD	N 2	LOFTHUS, A	60	600568
DHD	N 2	BROOK, M KAPLAN, J	54	600571
DHD	N 2	CARIO, G REINECKE,	50	600573
DHD	N 2	DOUGLAS, A HERZBER	51	600577
DHD	N 2	FARBER, M DARNELL	53	600579
DHD	N 2	HENDRIE, J	55	600582
DHD	N 2	LINDHOLM, E	54	600590
DHD	N 2	TOENNIES, J GREENE	57	600600
H	N 2	BOND, W	60	600664
PHAS	N 2	PANNETIER, G MARSI	61	600850
SPK	N 2	PANNETIER, G MARSI	61	600850
SPK	N 2	CARROLL, P	63	301424
SPK	N 2	CARROLL, B SAYERS	53	600545
SPK	N 2	WOLFSBERG, M	53	600546
SPK	N 2	BRYAH, R HOLT, R	57	600549
SPK	N 2	NICHOLLS, R REEVES	59	600562
SPK	N 2	WATANABE, K MARMO	56	600567
SPK	N 2	LOFTHUS, A	60	600568
SPK	N 2	ASTOIN, N GRANIER	57	600569
SPK	N 2	BRANSCOMB, L	51	600570
SPK	N 2	CARROLL, P RUBALCA	59	600572
SPK	N 2	CARIO, G REINECKE	50	600573
SPK	N 2	CARROLL, B	58	600574
DHD	N 2	CHRISTIAN, R DUFF	55	600575
SPK	N 2	CARROLL, B ROBALEA	60	600693
SPK	N 2	BAER, P MIESCHER	52	600729
SPK	N 2	DOUGLAS, A	52	600576
SPK	N 2	DRESSLER, K	59	600578
SPK	N 2	FEAST, M	51	600580
SPK	N 2	GRIIN, A	55	600581
SPK	N 2	HENDRIE, J	55	600582
SPK	N 2	HEPNER, G HERMAN	57	600583
SPK	N 2	HERMAN, L HERMAN	52	600584
SPK	N 2	HERMAN, R WENIGER	52	600585
SPK	N 2	HERMAN, R	52	600586

SPK	N 2	JANIN, J	50	600587
SPK	N 2	KISTIAKOWSKY, G WA	58	600588
SPK	N 2	LEBLANC, F TANAKA	58	600589
SPK	N 2	LOFTHUS, A	56	600591
SPK	N 2	LOFTHUS, A	57	600592
SPK	N 2	LOFTHUS, A MULLIKE	57	600593
SPK	N 2	MUSCHLITZ, E GOODM	53	600594
SPK	N 2	OGAWA, M TANAKA, Y	59	600595
SPK	N 2	OGAWA, M TANAKA, Y	60	600596
SPK	N 2	SAYERS, D CARROLL	53	600597
SPK	N 2	STOICHEFF, B	54	600598
SPK	N 2	TANAKA, Y	55	600599
SPK	N 2	VANDERSLICE, J MAS	59	600601
SPK	N 2	WILKINSON, P	57	600602
SPK	N 2	WILKINSON, P MULLI	57	600603
SPK	N 2	WILKINSON, P	60	600604
SPK	N 2	WILKINSON, P	59	600605
SPK	N 2	WORLEY, R	53	600606
SPK	N 2	DIELSE, G HEATH, D	60	600618
THER	N 2	WILLIAMS, N N	61	700669
SPK	N 2	BAER, P MIESCHER	53	600730
THER	N H 3	PHILLIPS, J WHITE	52	600892
DH	N O	KOERNER, W DANIELS	52	600745
DHO	N O	BROOK, M KAPLAN, J	54	600571
SPK	N O	BAER, P MIESCHER	52	600729
SPK	N O	BAER, P MIESCHER	53	600730
SPK	N O	BAER, P MIESCHER	51	600728
SPK	N O	PALIK, E RAO, K	56	600717
SPK	N O	TANAKA, Y	54	600683
SPK	N O	FLETCHER, W BEGUN	57	600763
SPK	N O	UEDA, M	55	600762
SPK	N O	THOMPSON, H GREEN	56	600761
SPK	N O	TANAKA, Y SEYA, M	51	600760
SPK	N O	SHAW, J	56	600759
SPK	N O	OGAWA, M	53	600758
SPK	N O	OGAWA, M	55	600757
SPK	N O	TANAKA, Y	54	600756
SPK	N O	OGAWA, M	55	600755
SPK	N O	NICHOLS, N HAUSE	55	600754
SPK	N O	MIGEOTTE, P ROSEN	45	600752
SPK	N O	MIGEOTTE, P ROSEN	50	600753
SPK	N O	MIGEOTTE, P	45	600751
SPK	N O	NICHOLLS, R	62	601625
SPK	N O	MIESCHER, E	56	600750
SPK	N O	MIESCHER, E	55	600749
SPK	N O	MARYOTT, A KRYDER	59	600748
SPK	N O	MARMO, F	53	600747
SPK	N O	LAGERQVIST, A MIES	58	600746
SPK	N O	HERZBERG, G LAGERQ	56	600744
SPK	N O	GALLAGHER, J KING	55	600743
SPK	N O	GALLAGHER, J JOHNS	56	600742
SPK	N O	GALLAGHER, J BEDAR	54	600741
SPK	N O	FEAST, M	50	600740
SPK	N O	DEEZSI, I MATRIN	57	600739
SPK	N O	DEEZSI, I	58	600738
SPK	N O	DEEZSI, I	56	600737
SPK	N O	BURRUS, C GRAYBEAL	58	600736
SPK	N O	BURRUS, C GORDY, W	53	600735
SPK	N O	BERINGER, R RAUSON	54	600734
SPK	N O	BARROW, R MIESCHER	57	600733
SPK	N O	SUTCLIFFE, L WALSH	53	600732
THER	N O	BIGELEISEN, J	60-	600799
VAP	N O	BIGELEISEN, J	60	600799
SPK	N O	BAER, P MIESCHER	53	600730
SPK	N 2O	PALIK, E RAO, K	56	600717
SPK	N 2O	RANK, D EASTMAN, D	61	600835
SPK	N 2O	TIDWELL, E	60	600921
CPH	N 2O 4	HISATSUME, J	59	600807
S	N 2O 4	HISATSUME, J	59	600807
SPK	N 2O 4	JACAB, J	59	600808
SPK	N 2O 4	HISATSUME, J	59	600807
ZKP	N 2O 4	JACOB, J	59	600808
BIB	NITRIDES	EHL, R	59	201141
CEMP	NITRIDES	KUBASCHENSKI, O	56	601642
CEMP	NITRIDES	GOODMAN, P HOMONOF	61	301460
CEMP	NITRIDES	SCLAR,N	61	300682
MISC	NITRIDES	STRASHINSKAYA, L	62	201790
MPP	NITRIDES	POPOVA, O KABANNIK	62	300960

REV	NB	BARTLETT, E SCHMID	61	701052
REV	NB	WOHLL, M	60	701053
REV	NB	HARRIS, W	61	201239
REV	NB	DOUGLAS, D KUNZ, F	61	300419
REV	NB	PECKNER, D	61	201307
REV	NB	SYRE, R	61	201579
S	NB	CLUSIUS, K FRANZOS	60	700987
SPK	NB	KORSUNSKII, M GENK	60	201274
SPK	NB	HOLLIDAY, J	61	201226
SPK	NB	SHADMI, Y	61	700954
SPK	NB	ROSENZWEIG, N PORT	60	700996
SPK	NB	SWEENEY, W SEAL, R	61	201112
SPK	NB	KORSUNSKIY, M GENK	60	400616
SURF	NB	COST, J	62	201781
TCON	NB	CONNOLY, A MENDELS	62	201536
TCON	NB	TYE, R	61	201117
THEO	NB	ROSENZWEIG, N PORT	60	700996
THEO	NB	FRANK, R	60	201284
THER	NB	SCHICK, H ANTHROP	63	300994
THER	NB	CARTER, W	61	601631
THER	NB	CARTER, W	62	300749
VAP	NB	BEAVIS, L	60	600659
PHAS	NB AL C	JEITSCHKO, W NOWOT	63	301485
PHAS	NB ALLOYS	RICHER, H WINCIERZ	62	201766
THER	NB B	MEERSON, G	60	300298
H	NB B 2	MEZAKI, R TILLEUX	62	601617
MPP	NB B 2	MALYUCHKOV, O POVI	62	202096
S	NB B 2	MEZAKI, R TILLEUX	62	601617
SPK	NB B 2	KORSUNSKII, M GENK	60	201274
THER	NB B 2	SCHICK, H ANTHROP	63	301580
CRYS	NB3B 2	KIEFFER, B BENESOV	58	600619
PHAS	NB B SYST	NOWOTNY, H BENESOV	59	201339
REAC	NB B SYST	SAMSONOV, G STRASH	62	300990
PHAS	NB B SI ALLOYS	NOWOTNY, H BENESOV	60	201765
DH	NB BR5	GROSS, P HAYMAN, C	62	300706
DH	NB BR5	SHCHUKAREV, S SIMI	62	201748
DH	NB BR O SYST	SHCHUKAREV, S SIMI	62	201748
CEMP	NB C	BONDARENKO, B ERMA	62	301409
CPH	NB C	KUSENKO, F GELD, P	59	300929
CPH	NB C	GELD, P KUSENKO, F	60	600803
CRYS	NB C	STORMS, E KRIKORIA	60	700980
CRYS	NB C	STORMS, E KRIKORIA	60	700979
VAP	NB C	FESENKO, V BOLGAR	63	301216
DH	NB C	MAH, A BOYLE, B	55	301297
REAC	NB C	SAEKI, Y OMORI, G	63	301339
CRYS	NB C	KEMPTER, C STORMS	60	701008
CRYS	NB C	ELLIOT, R KOMJATH	60	600621
CRYS	NB C	KEMPTER, C STORMS	63	201053
CRYS	NB C	STORMS, E KRIKORIA	60	600645
DH	NB C	KORNILOV, A LEONID	62	300923
DHD	NB C	BITTNER, H GORETZK	62	301132
H	NB C	GELD, P KUSENKO, F	60	600803
CEMP	NB C	BITTNER, H GORETZK	62	202004
MPP	NB C	GIORGI, A SZKLARZ	63	202039
KIN	NB C	KIRILLOVA, G MEERS	60	200759
PHAS	NB C	NADLER, M KEMPTER	60	700903
PHAS	NB C	STORMS, E KRIKORIA	60	700980
PHAS	NB C	SHAFFER, P	61	700941
PHAS	NB C	NORTON, J	60	701001
PHAS	NB C	BENESOVSKY E RUDY	61	100181
PHAS	NB C	NADLER, M KEMPTER	60	300301
REAC	NB C	SAMSONOV, G	[illegible]	301571
S	NB C	KAUFMAN, L	62	300910
SPK	NB C	KORSUNSKII, M GENK	60	201274
THER	NB C	SCHICK, H ANTHROP	63	301579
THER	NB C	BOLGAR, A	61	700938
TRT	NB C	MATTHIAS, B	61	300945
VAP	NB C	FRIES, R	62	601478
CEMP	NB C	SAMSONOV, G FOMENK	63	202128
VAP	NB C	BOLGAR, A	61	700938
CRYS	NB2C	ELLIOT, R KOMJATH	60	600621
THER	NB2C	SCHICK, H ANTHROP	63	301579
DH	NB CARBIDES	HUBER, E	61	201192
DH	NB CARBIDES	KUSENKO, F GELD, P	60	701007
REAC	NB CARBIDES	MEERSON, G ZELIKMA	61	201912
SURF	NB CARBIDES	FOMENKO, V	61	201420
PHAS	NB C SYST	ELLIOTT, R	62	301441
THER	NB C SYST	CUNNINGHAM, G WARD	63	301208

PHAS	NB C SYST	ELLIOTT, R	61	300262
PHAS	NB C SYST	ELLIOT, R KOMJATHY	60	301065
PHAS	NB C SYST	GELD, P LIUBIMOV	61	300380
PHAS	NB C SYST	KIMURA, H SASAKI	61	601578
PHAS	NB C SYST	KOVALCHENKO, M SAM	61	201472
REAC	NB C SYST	SAMSONOV, G STRASH	62	300990
REAC	NB C SYST	PORTNOI, K LEVINSK	61	300216
VAP	NB C SYST	FRIES, R	62	300591
REAC	NB C O SYST	STEVENS, E WILHELM	61	301597
REAC	NB C O SYST	SHVEIKIN, G GELD	63	301367
KIN	NB C O SYST	SHVEIKIN, G	58	301366
PHAS	NB C FE SYST	BELIKOV, A SAVINSK	62	300863
REAC	NB C W SYST	EVSTYUKHIN, A NIKI	62	300883
THER	NB CL	SCHAFER, H KAHLENB	60	200820
DF	NB CL5	JERE, G PATEL, C	60	200850
DH	NB CL5	SHCHUKAREV, S ORAN	60	200944
SPK	NB CL5	BADER, R	61	201260
PHAS	NB CL O SYST	MEYER, G OOSTEROM	61	201213
PHAS	NB H SYST	ELLIOTT, R KOMJATH	60	600621
MISC	NB MO SYST	BRAUN, H SEDLATSCH	60	200806
ERES	NB MO SYST	HULM, J BLAUGHER	61	201421
PHAS	NB MO C SYST	RUDY, E BENESOVSKY	61	300449
PHAS	NB MO V	BARON, V IVANOVA	60	200918
PHAS	NB MO W	SAVITSKII, E BARON	62	201705
CEMP	NB N	SAMSONOV, G FOMENK	63	202128
CRYS	NB N	KORSUNSKII, M GENK	63	301274
MPP	NB N	SAMSONOV, G VERKHO	61	301573
THER	NB N	BOLGAR, A	61	700938
VAP	NB N	SAMSONOV, G VERKHO	61	301569
VAP	NB N	BOLGAR, A	61	700938
S	NB N	KAUFMAN, L	62	300910
CEMP	NB N	KORSUNSKII, M GENK	62	300912
TRT	NB N	MATTHIAS, B	61	300945
MPP	NB N	SAMSONOV, G VERKHO	62	300997
CRYS	NB2N	ELLIOT, R KOMJATH	60	600621
CRYS	NB4N 3	ELLIOT, R KOMJATH	60	600621
PHAS	NB NITRIDES	BRAUER, G	61	201142
SPK	NB NITRIDES	KORSUNSKII, M GENK	60	201274
PHAS	NB NITRIDES	BRAUER, G	60	201037
CEMP	NB NITRIDES	SAMSONOV, G	60	700947
DH	NB NITRIDES	SAMSONOV, G	60	700947
REV	NB NITRIDES	SAMSONOV, G	60	700947
CTEX	NB N SYST	SAMSONOV, G VERKHO	61	601576
PHAS	NB N SYST	BRAUER, G ESSELBOR	61	700575
VAP	NB N SYST	COST, J WERT, C	62	300681
PHAS	NB N SYST	ELLIOT, R KOMJATHY	60	301065
PHAS	NB N SYST	ELLIOTT, R KOMJATH	60	600621
ERES	NB N SYST	SAMSONOV, G VERKHO	61	601576
VAP	NB N SYST	COST, J WERT, C	63	301432
VAP	NB N SYST	SAMSONOV, G VERKHO	61	601576
CRYS	NB N 2 SYST	ELLIOTT, R KOMJATH	61	701063
PHAS	NB N 2 SYST	ELLIOTT, R KOMJATH	61	701063
CRYS	NB O	BRAUER, G MORAWIET	62	301106
CRYS	NB O	HOCH, M	63	301477
CRYS	NB O	BRAUER, G MORAWIET	62	301414
CRYS	NB O	NORIN, R MAGNELI	60	200781
DF	NB O	HOCH, M	60	300311
EMF	NB O	LAVRENTEV, V GERAS	61	701030
REAC	NB O	LAVRENTEV, V GERAS	61	701030
REAC	NB O	HICKS, W	61	201011
REAC	NB O	SAZHIN, N KOLCHIN	61	300381
REAC	NB O	GORDON, G SCHEVERM	60	201499
REAC	NB O	KOLSKI, T	62	201497
REAC	NB O	GURI EV, T	61	201792
CPH	NB O	KUSENKO, F GELD, P	59	300929
CRYS	NB O	BRAUER, G MORAWIET	62	601681
MSP	NB O	SHCHUKAREV, S SEME	62	301354
SPK	NB O	UHLER, U	55	301370
S	NB O	KAUFMAN, L	62	300910
SPK	NB O	UHLER, U	54	600915
SPK	NB O	GRAVEN, W SALOMON	60	200911
THER	NB O	HOCH, M	61	301476
THER	NB O	SCHICK, H ANTHROP	63	301580
THER	NB O	LAVRENTEV, V GERAS	61	701030
THER	NB O	PEMSLER, J P	61	700660
TRT	NB O	KOLCHIN, O SUMAROK	61	600873
TRT	NB O	ELLIOT, R KOMJATH	60	600621
TRT	NB O	ELLIOT, R	60	600626

VAP	NB O	LAVRENTEV, V GERAS	61	701030
CPH	NB O 2	KUSENKO, F GELD, P	62	300727
CPH	NB O 2	KUSENKO, F GELD, P	59	300929
CPH	NB O 2	GELD, P KUSENKO, F	60	600803
CRYS	NB O 2	MARINDER, B O	61	700649
DH	NB O 2	KUSENKO, F GELD, P	62	300727
DH	NB O 2	MOROZOVA, M STOLYA	60	300186
EMF	NB O 2	LAVRENTEV, V GERAS	61	701030
H	NB O 2	GELD, P KUSENKO, F	60	600803
H	NB O 2	KING, E CHRISTENSE	61	600826
REAC	NB O 2	KUSENKO, F GELD, P	60	200823
REAC	NB O 2	LAVRENTEV, V GERAS	61	701030
S	NB O 2	KING, E CHRISTENSE	61	600826
THER	NB O 2	LAVRENTEV, V GERAS	61	701030
TRT	NB O 2	KOLCHIN, O SUMAROK	61	600873
TRT	NB O 2	ELLIOT, R KOMJATH	60	600621
TRT	NB O 2	ELLIOT, R	60	600625
VAP	NB O 2	LAVRENTEV, V GERAS	61	701030
VAP	NB O 2	GOLUBTSOV, I LAPIT	60	701029
VAP	NB O 2	SHCHUKAREV, S SEME	62	300744
THER	NB O 2	SCHICK, H ANTHROP	63	301580
SPK	NB O 5	CONLON, D DOYLE, W	61	201325
PHAS	NB2O	BRAUER, G MUELLER	58	301197
KIN	NB2O 3	SHVEIKIN, G GELD	60	200762
PHAS	NB2O 5	DIAMOND, J SCHNEID	60	202028
ERES	NB2O 5	MANALOV, P ESIN, O	62	202096
CRYS	NB2O 5	NORIN, R	63	202110
REAC	NB2O 5	GELD, P LYUBIMOV	62	301223
ERES	NB2O 5	GREENER, E FEAR, G	63	301232
CEMP	NB2O 5	JANNINCK, R WHITMO	63	301254
ERES	NB2O 5	JANNINCK, R	63	301255
REAC	NB2O 5	KIMURA, H SASAKI	62	301262
ERES	NB2O 5	KOFSTAD, P	62	301267
PHAS	NB2O 5	KOFSTAD, P	61	301268
ZKP	NB2O 5	LYUBINOV, V GELD	61	301294
ERES	NB2O 5	MAKKAY, R FINE, M	62	301298
ERES	NB2O 5	REISMAN, A HOLTZBE	59	301328
PHAS	NB2O 5	ZVINCHUK, R	58	301385
CEMP	NB2O 5	GRUNER, E WHITMORE	61	700527
CPH	NB2O 5	GELD, P KUSENKO, F	60	600803
CPH	NB2O 5	KUSENKO, F GELD, P	59	300929
CPH	NB2O 5	KUSENKO, F GELD, P	62	300727
CRYS	NB2O 5	KOFSTAD, P KJOLLES	61	701034
CRYS	NB2O 5	MARINDER, B	62	601678
CRYS	NB2O 5	LAKHIANI, D SHREIR	60	700978
DH	NB2O 5	KORNILOV, A LEONID	62	601591
DH	NB2O 5	KUSENKO, F GELD, P	62	300727
DH	NB2O 5	MOROZOVA, M P STOL	60	300186
DH	NB2O 5	KUSENKO, F G GELD	60	300252
EMF	NB2O 5	LAVRENTEV, V GERAS	61	701030
ERES	NB2O 5	GREENER, E WHITMOR	60	600631
ERES	NB2O 5	GRUNER, E WHITMORE	61	700527
H	NB2O 5	GELD, P KUSENKO, F	60	600803
KIN	NB2O 5	MOROZOV, I STEFANY	58	200796
KIN	NB2O 5	GELD, P SHVEIKIN	60	200996
PHAS	NB2O 5	GOLDSCHMIDT, H	60	200765
PHAS	NB2O 5	ROTH, R WARING, J	61	201406
REAC	NB2O 5	SHVEIKIN, G P	58	300151
REAC	NB2O 5	LAVRENTEV, V GERAS	61	701030
REAC	NB2O 5	LINBIMOV, V GELD	61	300388
THER	NB2O 5	KORNILOV, A LEONID	62	601591
THER	NB2O 5	SCHICK, H ANTHROP	63	301580
THER	NB2O 5	LAVRENTEV, V GERAS	61	701030
VAP	NB2O 5	LAVRENTEV, V GERAS	61	701030
VAP	NB2O 5	GOLUBTSOV, I LAPIT	60	701029
DH	NB OXIDES	KUSENKO, F GELD, P	60	701007
REAC	NB OXIDE	BRAUER, G MULLER		300561
THER	NB OXIDES	ORTNER, N ANDERSON	59	701066
VAP	NB OXIDES	ORTNER, N ANDERSON	59	701066
KIN	NB O SYST	HURLEN, T KJOELLES	59	201306
MPP	NB O SYST	ALYAMOVSKIY, G SHV	58	400597
PHAS	NB O SYST	KUSENKO, F GELD, P	61	201116
MPP	NB O SYST	GEBHARDT, E ROTHEN	63	202036
KIN	NB O SYST	HURLEN, T	60	301250
VAP	NB O SYST	SHCHUKAREV, S SEME	59	301353
PHAS	NB O SYST	SHVEIKIN, G GELD	58	301356
PHAS	NB O SYST	BRAUER, G MUELLER	63	301196
PHAS	NB O SYST	BRAUER, G MUELLER	62	301413

PHAS	NB O SYST		
	ELLIOTT, R	62	301441
PHAS	NB O SYST		
	BRAUER, G MUELLER	62	301413
PHAS	NB O SYST		
	TERAO, N	63	301603
PHAS	NB O SYST		
	KOUBA, L TRUNOV, V	62	301278
PHAS	NB O SYST		
	GRIGOREVA, N SELEZ	62	300888
PHAS	NB O SYST		
	ELLIOT, R	60	600625
PHAS	NB O SYST		
	ELLIOT, R KOMJATHY	60	301055
PHAS	NB O SYST		
	NORMAN, N	62	300374
PHAS	NB O SYST		
	BRAUER, G ESSELBOR	61	201114
PHAS	NB O SYST		
	ELLE, M CHIPMAN, J	61	300281
PHAS	NB O SYST		
	NORMAN, N KOFSTAD	62	300527
REAC	NB O SYST		
	ARGENT, B PHELPS	60	600611
THER	NB O SYST		
	MEERSON, G	62	300946
ZKP	NB O SYST		
	KUSENKO, F GELD, P	61	201116
REAC	NB O C SYST		
	SHVEYKIN,G	58	600672
THER	NB O C SYST		
	SHVEYKIN,G	58	600671
ZKP	NB O C SYST		
	KUSENKO, F GELD, P	61	700619
ZKP	NB O C SYST		
	SHVEYKIN,G	58	600671
KIN	N O H SYST		
	BLACKBURN, P	62	301189
ZKP	NB O H SYST		
	LINBIMOV, V GELD	61	300388
PHAS	NB O N SYST		
	ELLIOTT, R KOMJATH	60	600621
PHAS	NB PD SYST		
	SAVITSKII, E BARON	61	201429
PHAS	NB RE SYST		
	KAUFMANN A R RAPPR	61	300218
PHAS	NB RE SYST		
	GIESSEN, W NORDHEI	61	201233
PHAS	NB SI		
	ALYAMOUSKII, P GEL	61	201586
PHAS	NB SI O SYST		
	IBRAHIM, M BRIGHT	62	201638
REAC	NB TA		
	SCHAEFER, H HUEESK	62	201959
PHAS	NB TE SYST		
	GRIGORYAN, L SIMAN	60	200992
KIN	NB TI SYST		
	VOITOVICH, R	61	201287
PHAS	NB TI TA SYST		
	KORNILOV, M PYLAEV	61	300508
PHAS	NB TI ZR SYST		
	MIKHEEV, V BELOUSO	61	300834
PHAS	NB U C SYST		
	BENESOVSKY, F RUDY	61	301406
MISC	NB W SYST		
	BRAUN, H SEDLATSCH	60	200806
KIN	NB ZR SYST		
	VOITOVICH, R	61	201287
PHAS	NB ZR SYST		
	LUNDIN, C	61	201120
CPH	ND		
	ARAJS, S COLVIN, R	62	300751
CPH	ND		
	SPEDDING, F MILLER	51	601241
CPL	ND		
	GOODMAN, B	52	100208
CPL	ND		
	PARKINSON, D H SIM	51	400557
CRYS	ND		
	ELLINGER, F	53	601253
CRYS	ND		
	ELLINGER, F	55	600977
DH	ND		
	JOHNSON, R	56	601293
DH	ND		
	WHITE, D	61	201217
CTEX	ND		
	ANDRES, K	63	301172
DH	ND		
	JOHNSON, R HUDSON	52	601224
DH	ND		
	AMES LABORATORY	52	601247
DH	ND		
	HUBER, J	52	100213
ERES	ND		
	ALSTAD, J COLVIN	61	201099
ERES	ND		
	SPEDDING, F DAANE	57	601066
ERES	ND		
	BRIDGMAN, P	51	400533
ERES	ND		
	GOODMAN, B	52	100208
ERES	ND		
	JAMES, N LEGNOLD	52	100206
H	ND		
	SPEDDING, F MILLER	51	601241
MPP	ND		
	IOWOV, W MITTSEV	60	601332
MSP	ND		
	JOHNSON, R HUDSON	56	601040
MSP	ND		
	JOHNSON, R HUDSON	52	601224
PHAS	ND		
	SPEDDING, F DAANE	57	601066
PHAS	ND		
	JOHNSON, R HUDSON	56	601040
PHAS	ND		
	SPEDDING, F DAANE	57	700872
PHAS	ND		
	JOHNSON, R	56	601293
PHAS	ND		
	TROMBE, F FOEY, M	51	400546
SPK	ND		
	NOLDEKE, G	55	601028
SPK	ND		
	BURBRIDGE, E BURBR	55	601003
SPK	ND		
	KOROLEV, F	56	601321
SPK	ND		
	MURAKAWA, K	54	601284
SPK	ND		
	SCHWARZSCHILD, M	57	601047
SPK	ND		
	SMITH, K SPALDING	62	300777
SPK	ND		
	HOVIS, W	62	300824
SPK	ND		
	GARSTANG, R	52	100207
SPK	ND		
	VAN DIJKE BEATTY, S	51	400548
SPK	ND		
	TAKEHIKO, I SHIN Y	50	400552
SPK	ND		
	GRATTON, I	52	400567
SPK	ND		
	BLAISE, J	58	601123
SPK	ND		
	IONOV, N MITKEV, M	60	601180
THER	ND		
	PARKINSON, D H SIM	51	400557
THER	ND		
	SPEDDING, F H MCKE	60	700570
TRT	ND		
	JOHNSON, R HUDSON	56	601040
TRT	ND		
	TROMBE, F FOEX, M	51	400546

VAP	ND	YAMAMOTO, A S LUND	61	300230
VAP	ND	JOHNSON, R	56	601293
VAP	ND	WHITE, D WALSH, P	61	301014
VAP	ND	JOHNSON, R HUDSON	52	601224
VAP	ND	WHITE, D WALSH, P	60	301622
VAP	ND	AMES LABORATORY	52	601247
VAP	ND	WHITE, D WALSH, P	61	300455
SPK	ND+	JUDD, B	55	600927
SPK	ND+	NOLDEKE, G STEUDEL	54	600931
SPK	NDI	NOLDEKE, G STEUDEL	54	600952
SPK	ND2	BURBRIDGE, G BURBR	54	600937
CEMP	ND B 6	SAMSONOV, G PADERN	59	300143
CRYS	ND B 6	SAMSONOV, G PADERN	60	601382
PHAS	ND C SYST	WARF, J PALENIK, G	60	600636
PHAS	ND CE MG SYST	ROKHLIN, L	62	201703
VAP	ND CL3	NOVIKOV, G BAEV, A	62	300686
CRYS	ND N SYST	IANDELLI, A	38	601275
CRYS	ND O	ELLINGER, F	53	601253
VAP	ND O	TROMBE, F FOEX, M	63	301367
DHD	ND O	GOLDSTEIN, H WALSH	58	201098
DHD	ND O	GOLDSTEIN, H	61	201216
VAP	ND O	KULVARSHAYA, B MAS	60	301064
VAP	ND O	GOLDSTEIN, H WALSH	61	700889
CPH	ND2O 3	PANKRATZ, L KING	62	300958
CPH	ND2O 3	GOLDSTEIN, H NGILS	59	601198
CPH	ND2O 3	BLOMEKE, J O ZIEGL	51	400562
CPL	ND2O 3	GOLDSTEIN, H	58	601551
CPL	ND2O 3	GOLDSTEIN, H NEILSO	60	700836
CPL	ND2O 3	JUSTICE, B WESTRUM	63	300906
CRYS	ND2O 3	DOUGLASS, R	56	601010
H	ND2O 3	BLOMEKE, J O ZIEGL	51	400562
MSP	ND2O 3	PANISH, M	61	601372
REAC	ND2O 3	KELER, E GODINA, N	61	300387
S	ND2O 3	BLOMEKE, J O ZIEGL	51	400562
THER	ND2O 3	BLOMEKE, J O ZIEGL	51	400562
VAP	ND2O 3	GOLDSTEIN, H WALSH	60	700889
VAP	ND2O 3	GOLDSTEIN, H WALSH	58	201098
VAP	ND2O 3	PANISH, M	61	601372
VAP	ND2O 3	GOLDSTEIN, H	57	601489
VAP	ND2O 3	GOLDSTEIN, H	60	201018
VAP	ND2O 3	GOLDSTEIN, H	61	201216
DH	ND O SYST	WALSH, P N DEVER	61	700642
PHAS	ND O SYST	POPOV, A GLOCKER	49	400524
PHAS	NI MO CR SYST	ZAKHAROVA, M PROKO	61	201241
MPP	NONSTOICHIOMETRY	LAZARUS, D	62	301518
REV	NONSTOICHIOMETRY	SEEGER, A	61	301586
REV	NONSTOICHIOMETRY	ANDERSON, J	63	301396
THEO	NONSTOICHIOMETRY	WADSLEY, A	63	301615
ZKP	NONSTOICHIOMETRY	ELLIOTT, G LEMONS	63	301440
SPK	NUCLEI	BELYAEV, S	61	700550

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PHAS	O	BEREZHNOI, A KORDY	62	201553
PHAS	O	WYDER, W HOCH, M	62	201581
SPK	O	MALTSEV, A KATAEV	60	600701
SPK	O	PILCHER, G SKINNER	62	301044
THER	O	ACKERMANN, R THORN	58	601208
MISC	O	LADD, M LEE, W	60	201322
MPP	O	REVYAKIN, A	61	201286
CPH	O 2	WILLIAMS, N N	61	700659
DHD	O 2	BRIX, B HERZBERG	53	600544
DHD	O 2	LOSEV, S GENERALOV	61	300583
DHD	O 2	BRIX, B HERZBERG	54	600548
DHD	O 2	CAMAC, M VAUGHAN	59	600613
REV	O 2	HERZBERG, G	52	600536
SPK	O 2	HERZBERG, G	52	600536
SPK	O 2	HERZBERG, G	53	600537
SPK	O 2	MOFFITT, W	51	600539
SPK	O 2	WEBER, A MCGINNIS	60	600540
SPK	O 2	BARTH, C KAPLAN, J	59	600541
SPK	O 2	CHAMBERLAIN, J	58	600542
SPK	O 2	WILKINSON, B MULLI	57	600543
SPK	O 2	BRIX, P HERZBERG	53	600544
SPK	O 2	BROIDA, H GAYDON	54	600547
SPK	O 2	BRIX, B HERZBERG	54	600548
SPK	O 2	BRYAH, R HOLT, R	57	600549
SPK	O 2	BURKHALTER, J ANDE	60	600550

SPK	O 2	BURKHALTER, J ANDE	50	600551
SPK	O 2	CARROLL, P	59	600552
SPK	O 2	FEAST, M	49	600553
SPK	O 2	FEAST, M	50	600554
SPK	O 2	HERMAN, R HERMAN	49	600555
SPK	O 2	HERMAN, R WENIGER	50	600556
SPK	O 2	HERMAN, R HERMAN	50	600557
SPK	O 2	HERMAN, R WENIGER	50	600558
SPK	O 2	MILLER, S TOWNES	53	600559
SPK	O 2	MILLER, S TOWNES	53	600560
SPK	O 2	MILLER, S TOWNES	53	600561
SPK	O 2	NICHOLLS, R REEVES	59	600562
SPK	O 2	TANAKA, Y	52	600563
SPK	O 2	TANAKA, Y JURSA, A	56	600564
SPK	O 2	WATANABE, K INN, E	53	600566
SPK	O 2	WATANABE, K MARMO	56	600567
SPK	O 2	CAMAC, M VAUGHAN	59	600613
SPK	O 2	ZIMMERER R MIZUSH	61	600920
SPK	O 2	LOSEV, S GENERALOV	61	301113
THER	O 2	WILLIAMS, N N	61	700659
MPP	ORGANICS	DREISBACH, R	61	300263
BIB	OS	ANON	60	701024
COPT	OS	DOUGLAS, R W ADKIN	61	700614
MPP	OS	FRANCIS, A	62	301076
CRYS	OS	MCCALDIN, J DUWEZ	54	600956
PHAS	OS	KNAPTON, A SAVILL	60	600663
PHAS	OS	SAVITSKII, E TYLKI	63	301575
PHAS	OS	KNAPTON, A SAVILL	60	700995
PHAS	OS	DOUGLAS, R W ADKIN	61	700614
REAC	OS	SPACU, P GHEORGHIV	61	201693
REAC	OS	SEMENOV, I KOLBIN	62	201486
SPK	OS	BARINSKI, R NADZHA	60	200910
SPK	OS	ROSENZWEIG, N PORT	60	700901
SPK	OS	VAN KLEEF, T	61	600656
SPK	OS	MURAKAWA, K SUWA	52	600942
SPK	OS	ROSENZWEIG, N PORT	60	700996
SPK	OS	VANKLEEF, T KLINK	61	701033
SPK	OS	HINES, A ROSS, J	62	601592
SPK	OS	VAN KLEEF, T	60	600692
SPK	OS	MOORE, C	58	601088
SPK	OS	VAN KLEEF, T KLINK	61	201113
SPK	OS	BLAISE, J	58	601123
THEO	OS	ROSENZWEIG, N PORT	60	700996
THEO	OS	ROSENZWEIG, N PORT	60	700901
THER	OS	BARRIAULT, R DREIK	62	300865
TRT	OS	KNAPTON, A SAVILL	60	201068
TRT	OS	KNAPTON, A SAVILL	60	600663
TRT	OS	MCCALDIN, J DUWEZ	54	600956
VAP	OS	HASAPIS, A PANISH	60	700994
VAP	OS	PANISH, M REIF, L	62	300721
REAC	OS BR3	SHCHUKAREV, S KOLB	61	201231
CRYS	OS B SYST	KEMPTER, C P FRIES	61	700621
CRYS	OS B SYST	KEMPTER, C P FRIES	61	700621
CRYS	OS B SYST	KEMPTER, C FRIES	61	701050
CRYS	OS B SYST	ARONSON, B STENBER	62	300757
CRYS	OS B SYST	KEMPTER, C FRIES	61	201103
MPP	OS B SYST	BUDDERY, J WELCH	51	600940
PHAS	OS B SYST	ROOF, R KEMPTER, C	62	300966
CRYS	OS C	KEMPTER, C NADLER	60	701010
PHAS	OS C	NADLER, M KEMPTER	60	300301
REAC	OS C	KEMPTER, C NADLER	60	201024
REAC	OS C	KEMPTER, C NADLER	60	201024
CEMP	OS F 6	EISENSTEIN, J	61	201126
SPK	OS F 6	EISENSTEIN, J	61	201126
REAC	OS I	FERGUSON, J ROBIN	62	201686
SPK	OS O	WOODWARD, L CREIGH	60	200760
THER	OS O	BARRIAULT, R DREIK	62	300865
THER	OS O 2	BARRIAULT, R DREIK	62	300865
THER	OS O 3	BARRIAULT, R DREIK	62	300865
THER	OS O 4	BARRIAULT, R DREIK	62	300865
PHAS	OS RE	TYLKINA, M POLYAKO	62	201728
PHAS	OS RU	TYLKINA, M POLYAKO	62	201729
PHAS	OS TA SYST	KAUFMANN, A R RAPPR	61	300218
PHAS	OS W SYST	KAUFMANN A R RAPPR	61	300218
THEO	OXIDATION	LEVINSON, M KOVROV	60	301100
THEO	OXIDATION	SEYBOLT, A	63	301350
CEMP	OXIDES	KUBASCHENSKI, O	56	601642
DHD	OXIDES	BERKOWITZ, J	59	301187

REAC	OXIDES	COLLONGUES, R GILL	63	301205
VAP	OXIDES	NOGA, K	62	301313
CEMP	OXIDES	VORONOV, N DANILIN	62	301120
CRYS	OXIDES	BAUR	61	200955
CRYS	OXIDES	SIDOROV, T	60	201055
CRYS	OXIDES	WADSLEY, A	61	201101
CTEX	OXIDES	TAYLOR, R	60	200793
CTEX	OXIDES	KUMAR, S	60	700685
DH	OXIDES	KAPUSTINSKII, A	48	600627
DH	OXIDES	KLYUCHNIKOV, N	60	300659
DH	OXIDES	SHARUPIN, B VASILK	61	700665
DHD	OXIDES	BREWER, L ROSENBLA	61	201111
E	OXIDES	MEN, A ORLOV, A	58	200794
KIN	OXIDES	OATS, TODD, D	62	201903
MSP	OXIDES	GRIMLEY, R BURNS	60	200817
PHAS	OXIDES	SIDEBOTTOM, B WHIT	61	201048
PHAS	OXIDES	ESTULIN, G EGORSHI	62	900207
PHAS	OXIDES	GOUTER, E W	59	700608
PHAS	OXIDES	SCHNEIDER, S ROTH	61	201407
PHAS	OXIDES	COCCO, A SCHROMEK	61	201637
REAC	OXIDES	MORIN, F	61	201273
REAC	OOXIDES	SAMSONOV, G YASINK	61	100180
REAC	OXIDES	BORCHARDT, H THOMP	60	200887
REAC	OXIDES	SAMSONOV, G IASINS	61	300340
REAC	OXIDES	TRIBALAT, S JUNGFL	60	200829
REV	OXIDES	BURKE, J	61	601403
REV	OXIDES	LANE, Z TUNIS, M	62	201940
SPK	OXIDES	SIDOROV, T	60	201055
SPK	OXIDES	VRATNY, F DILLING	61	201385
TCON	OXIDES	TAYLOR, R	60	200793
THEO	OXIDES	YATSIMIRSKII, K B	61	300180
THER	OXIDES	ACKERMANN, R J THO	61	700580
THER	OXIDES	HAHN, W	60	200812
THER	OXIDES	KUBASCHENSKI, O	56	601642
THER	OXIDES	BREWER, L	62	300855
THER	OXIDES	BREWER, L	63	700843
VAP	OXIDES	VORONOV, N DANILIN	62	300563
VAP	OXIDES	ACKERMANN, R J THO	61	700580
VAP	OXIDES	BURKE, J	61	601403
TRT	OXIDES	SCHNEIDER, S	63	202131

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THEO	PARTIAL MOLAR	KRESTOV, G	63	301283
THER	PB	MARGRAVE, J	61	700967
VAP	PB O	FIRSOVA, L NESEMEY	60	200761
CPL	PD	CRANGLE, J SMITH	62	300869
CPL	PD	BORELIUS, G	60	601168
dh	PD	GOLDSMITH, A HIRSC	60	700930
DHT	PD	LOWRIE, R	61	700943
MPP	PD	EREMENKO, V NAIDIC	61	300529
MPP	PD	FRANCIS, A	62	301076
PHAS	PD	GOLDSMITH, A HIRSC	60	700930
PHAS	PD	MENDENHALL, C INGE	07	900143
SPK	PD	SHADMI, Y	61	700954
SPK	PD	KESSLER, K MEGGERS	54	600976
TRT	PD	MENDENHALL, C INGE	07	900143
VAP	PD	DREGER, L MARGRAVE	60	200922
VAP	PD	GOLDSMITH, A HIRSC	60	700930
VAP	PD	DREGER, L	61	300528
VAP	PD	WALKER, R F EFIMEN	61	700579
CRYS	PD B SYST	ARONSON, B ASELIUS	59	601166
THEO	PHASE DIAGRAM	BREWER, L	63	202009
THEO	PHASE DIAGRAM	HUME, W ROTHERY	63	301249
THEO	PHASE RULE	BRYNESTAD, J	63	301199
THEO	PHASES	HERIC, E	63	202049
THEO	PHASES	MERTSLIN, R NIKURA	63	202102
THEO	PHASES	PAK, T KOGAN, V	62	202113
THEO	PHASES	PINAEV, G	63	202118
THER	PHASES	STORONKIN, A MORAC	63	202144
THER	PHASES	STORONKIN, A SMIRN	62	202145
MPP	POLYATOMIC GAS	GREEN, M	62	300636
SPK	POLYATOMIC GAS	HOUGEN, J	62	300781
THEO	POLYATOMIC GAS	KHACKKURUZOV, G MI	61	700547
THEO	POLYATOMIC GAS	KHACHKURUZOV, G MI	61	700677
THER	POLYATOMIC GAS	GODNEV, I	56	300832
THER	POLYATOMIC GAS	ARTYM, R	62	300773
THER	POLYATOMIC GAS	MCBRIDE, B GORDON	61	300473

THER	POLYATOMIC GAS	KHACHKURUZOV, G MI	61	700677
CPL	PR	GOODMAN, B	52	100208
CPL	PR	PARKINSON, D H SIM	51	400557
DH	PR	JOHNSON, R	56	601293
DH	PR	WHITE, D	61	201217
DH	PR	JOHNSON, R HUDSON	52	601224
DHT	PR	CAVALLERO, U	43	700895
ERES	PR	SPEDDING, F DAANE	57	601066
ERES	PR	BRIDGMAN, P	51	400533
ERES	PR	JAMES, N LEGNOLD	52	100206
ERES	PR	ALSTAD, J COLVIN	61	201099
ERES	PR	GOODMAN, B	52	100208
MPP	PR	IOWOV, W MITTSEV	60	601332
MSP	PR	JOHNSON, R HUDSON	52	601224
MSP	PR	JOHNSON, R HUDSON	56	601040
PHAS	PR	JOHNSON, R	56	601293
PHAS	PR	SPEDDING, F DAANE	57	601066
	PR	JOHNSON R HUDSON	56	601040
PHAS	PR	SPEDDING, F DAANE	57	700872
SPK	PR	GARSTANG, R	52	100207
SPK	PR	HOVIS, W	62	300824
SPK	PR	GRATTON, L	52	400567
SPK	PR	BURBRIDGE, E BURBR	55	601003
SPK	PR	IONOV, N MITKEV, M	60	601180
THER	PR	PARKINSON, D H SIM	51	400557
TRT	PR	JOHNSON, R HUDSON	56	601040
VAP	PR	YAMAMOTO, A S LUND	61	300230
VAP	PR	JOHNSON, R	56	601293
VAP	PR	WHITE, D WALSH, P	60	301622
VAP	PR	WHITE, D WALSH, P	61	300455
VAP	PR	WHITE, D WALSH, P	61	301014
VAP	PR	JOHNSON, R HUDSON	52	601224
SPK	PR	JUDD, B	55	600927
SPK	PR2	BURBRIDGE, G BURBR	54	600937
CEMP	PR B 6	SAMSONOV, G PADERN	59	300143
DF	PR C	DANCY, E EVERETT	62	300876
REV	PR C	ROUGH, F CHUBB, W	60	600610
VAP	PR CL3	NOVIKOV, G BAEV, A	62	300686
PHAS	PR C SYST	WARF, J PALENIK, G	60	600636
CRYS	PR N SYST	IANDELLI, A	37	601276
ERES	PR N SYST	DAOU, J	60	600615
THER	PROPELLANTS	SUNDARAM, S	63	301365
PHAS	PR O	EYRING, L HOLWBERG	62	601590
VAP	PR O	KULVARSHAYA, B MAS	60	301064
CRYS	PR O 2	GRUEN, D KOEHLER	61	400545
ERES	PR O 2	KEVANE, C	62	601467
PHAS	PR O 2	FAETH, P	61	701076
CRYS	PR2O 3	HONIG, J	58	601531
CRYS	PR2O 3	GRUEN, D KOEHLER	61	400545
MSP	PR2O 3	PANISH, M	61	601372
PHAS	PR2O 3	HONIG, J	58	601531
ERES	PR2O 3	HONIG, J	58	601531
REV	PR2O 3	HONIG, J	58	601531
VAP	PR2O 3	PANISH, M	61	601372
CPH	PR6O 11	BLOMEKE, J O ZIEGL	51	400562
H	PR6O 11	BLOMEKE, J O ZIEGL	51	400562
S	PR6O 11	BLOMEKE, J O ZIEGL	51	400562
THER	PR6O 11	BLOMEKE, J O ZIEGL	51	400562
BIB	PR OXIDES	JONES, P	60	200984
CRYS	PR O SYST	EYRING, L BAENZIGE	62	300825
DH	PR O SYST	WALSH, P N DEVER	61	700642
THER	PR O SYST	KUZNETSOV, F REZUK	62	300627
BIB	PT	WOHLL, M	60	700723
BIB	PT	GOODWIN, T	56	601547
CEMP	PT	WHITE, G WOODS, S	57	601050
CEMP	PT	CLUSIUS, K LOSA, C	57	601101
CPH	PT	CARTER, W	61	601631
CPH	PT	KENDALL, W ORR, R	62	601674
CPH	PT	DOUGLASS, R HOLDEN	59	700375
CPL	PT	RAMANATHAN, K SRIN	59	601132
CPL	PT	BORELIUS, G	60	601168
CRYS	PT	EDWARDS, J SPEISER	51	601179
CTEX	PT	CARTER, W	61	601631
CTEX	PT	EDWARDS, J SPEISER	51	601179
DH	PT	GOLDSMITH, A HIRSC	60	700930
DH	PT	HAMPSON, R WALKER	61	700681
ERES	PT	BRIDGMAN, P	51	400533
ERES	PT	HOPKINS, M	57	601171

H	PT	KENDALL, W ORR, R	62	601674
H	PT	RAMANATHAN, K SIRI	60	600697
KIN	PT	FRYBURG, G C PETRU	61	700596
MPP	PT	FRANCIS, A	62	301076
PHAS	PT	ORIANI, R JONES, T	54	600954
PHAS	PT	GOLDSMITH, A HIRSC	60	700930
PHAS	PT	HENNING, F WENSEL	33	900128
PHAS	PT	ROESER, W CALDWELL	31	900135
PHAS	PT	ROESER, W WENSEL	35	900134
PHAS	PT	WENSEL, H ROESER	34	900133
PHAS	PT	DAY, A SOSMAN, R	10	900137
PHAS	PT	MENDENHALL, C INGE	07	900143
PHAS	PT	JAFFEE, R MAYKUTH	60	201285
REAC	PT	LACROIX, R	56	601037
REAC	PT	FRYBURG, G C PETRU	61	700596
REAC	PT	BARTLETT, N LOHMAN	60	201810
REV	PT	CHASTON, J	50	600941
REV	PT	KLAUS, K	54	600973
SPK	PT	MOORE, C	58	601088
SPK	PT	KESSLER, K MEGGERS	54	600976
SURF	PT	KOZAKEVITCH, P URB	61	201558
TCON	PT	KRISHMAN, K	54	601281
REV	PT	BETTERIDGE, W RHYS	62	202003
TCON	PT	GERTSRIKEN, S	62	301454
TCON	PT	WHITE, G WOODS, S	57	601050
THER	PT	SCHICK, H ANTHROP	62	300995
THER	PT	CARTER, W	61	601631
THER	PT	GOODWIN, T	56	601547
THER	PT	CARTER, W	62	300749
THER	PT	DOUGLASS, R HOLDEN	59	700375
TRT	PT	HENNING, F WENSEL	33	900128
TRT	PT	ROESER, W CALDWELL	31	900135
TRT	PT	ROESER, W WENSEL	35	900134
TRT	PT	WENSEL, H ROESER	34	900133
TRT	PT	DAY, A SOSMAN, R	10	900137
TRT	PT	MENDENHALL, C INGE	07	900143
VAP	PT	DREGER, L MARGRAVE	60	200922
VAP	PT	HANLIN, H	60	700951
VAP	PT	GOLDSMITH, A HIRSC	60	700930
VAP	PT	DREGER, L	62	300720
VAP	PT	DREGER, L	61	300528
VAP	PT	DREGER, L MARGRAVE	60	600644
VAP	PT	HAMPSON, R WALKER	61	700681
MPP	PT BORIDES	POLKOVNIKOV, B BAL	62	300964
CRYS	PT BORIDES	ARONSSON, B STENBE	60	201349
CRYS	PT B SYST	ARONSON, B ASELIUS	59	601166
PHAS	PT B SYST	HUBBARD, F	59	601213
CRYS	PT C SYST	KONIG, H	51	600944
THER	PT O	SCHICK, H ANTHROP	62	300995
CRYS	PT O 2	GOCHE, O	51	600943
CRYS	PT O 2	SHISHAKOV, N	57	601121
THER	PT O 2	ALCOCK, C HOOPER	60	601161
DH	PT3O 4	ARIYA, S MOROZOVA	53	600970
THER	PT OXIDES	SHEWCHUCK, S	52	601252
CRYS	PT O SYST	BUSCH, R	50	600939
REV	PT O SYST	BUSCH, R	51	600945
THER	PT O SYST	SCHAFER, H TEBBEN	60	601159
DH	PU AL SYST	AKHACHINSKIY, V KO	62	301104
VAP	PU C	ANSELIN, F PASCARD	62	301126
DH	PU FE SYST	AKHACHINSKIY, V KO	62	301104
VAP	PU N	ANSELIN, F PASCARD	62	301126
PHAS	PU O U SYST	PIJONOWSHI, D DELU	60	600767
VAP	PULSE METHOD	PROTOPOPOV, N KULG	61	300718

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VAP	RADIATION	ZIMAKOV, I SPITSYN	61	300684
REV	RARE EARTHS	SPEDDING, F	62	301077
CEMP	RARE EARTHS	SIDAR, N	61	300233
CPL	RARE EARTHS	DREYFUS, B GOODMAN	61	300646
CRYS	RARE EARTHS	KOMKOV, A	59	201418
DH	RARE EARTHS	SEREBRENNIKOV, V	57	601131
MPP	RARE EARTHS	EFREMOV, N	54	600932
PHAS	RARE EARTHS	SAVITSKII, E LIVAN	61	201889
PREP	RARE EARTHS	LOVE, B	61	201690
REAC	RARE EARTHS	VEKSHINA, N MARKOV	61	201423
REAC	RARE EARTHS	CAMPBELL, T BLOCK	61	201328
REAC	RARE EARTHS	PICON, M DOMANGE	60	200790

REAC	RARE EARTHS	TEREKHOVA, V SAVIT	60	200833
REAC	RARE EARTHS	WARSHAW, I ROY, R	62	201808
REV	RARE EARTHS	WYLIE, A	50	400550
REV	RARE EARTHS	QUILL, L L	50	400553
SPK	RARE EARTHS	BERGVALL, P HAGSTR	60	601341
SPK	RARE EARTHS	MOORE, C	63	301538
THER	RARE EARTHS	BERG, J	62	201562
SPK	RARE EARTHS	BIDELMAN, W	53	100193
SPK	RARE EARTHS	CONNICK, R	49	400528
SPK	RARE EARTHS	TCHENG, MAO LIN	49	400584
SPK	RARE EARTHS	TCHENG, MAO LIN	50	400585
SPK	RARE EARTHS	KNISELEY, R FASSEL	59	601191
SPK	RARE EARTHS	HEORD, J F	50	400586
SPK	RARE EARTHS	SAKELLARDIS, P	55	600926
SPK	RARE EARTHS	JORGENSEN, C	55	600928
SPK	RARE EARTHS	BURBRIDGE, G BURBR	55	600929
SPK	RARE EARTHS	SAKELLARIDIS, P	55	600979
BOOK	RARE EARTHS	SAVITSKII, E TEREK	62	202129
SPK	RARE EARTHS	BOVEY, L STEERS, E	59	601190
SPK	RARE EARTHS	ROSE, A BLANDIN, J	60	201807
THER	RARE EARTHS	EMLEY, E	52	100209
THER	RARE EARTHS	BERG, J	62	300390
THER	RARE EARTHS	BAEV, A NOVIKOV, G	61	201410
VAP	RARE EARTHS	WHITE, D	60	300307
VAP	RARE EARTHS	BEAVIS, L	60	701016
VAP	RARE EARTHS	TROMBE, F	53	600960
ERES	RARE EARTHS	VERESHCHAGIN, L	61	201570
REV	RARE METALS	HAMPEL, C	54	600951
BIB	R E BORIDES	KLEBER, E	60	601450
CRYS	R E BORIDES	KLEBER, E	60	601450
CRYS	R.E BORIDES	ZHDANOV, G ZHURALE	60	200835
REAC	R E. BORIDES	PADERNO , Y B SAMS	60	300134
REV	R.E BORIDES	PADERNO, Y B SAMSO	60	300134
CRYS	R.E. BORIDES	NESHPOR, V SAMSONO	57	601107
CRYS	R.E. BORIDES	NESHPOR, V SAMSONO	58	601116
CRYS	R.E. BORIDES	LAFFERTY, J	51	400549
CRYS	R.E. BORIDES	EICK, H GILLES, P	59	601184
CRYS	R E. BORIDES	EICK, H	58	601537
ERES	R.E. BORIDES	SAMSONOV, V	61	700587
ERES	R.E. BORIDES	KLEBER, E	60	601450
MISC	R.E. BORIDES	PADERNO, Y FOMENKO	60	200933
MISC	R.E BORIDES	SAMSONOV, G PADERN	61	300317
MPP	R.E BORIDES	SAMSONOV, G	56	601255
MPP	R E BORIDES	NACHMAN, J LUNDIN	62	301539
MPP	R E. BORIDES	GAUME MAHN, F	56	601048
PHAS	R E. BORIDES	KLEBER, E	60	601450
REAC	R E. BORIDES	KUDINSTEVA, G EPLB	55	601182
REAC	R E BORIDES	KLEBER, E	60	601450
REV	R.E BORIDES	KLEBER, E	60	601450
REV	R.E BORIDES	GAUME MAHN, F	56	601048
BIB	R.E CARBIDES	KLEBER, E	60	601450
BIB	R E CARBIDES	ANON	58	601561
DH	R E CARBIDES	WENDLANDT, W GEORG	61	201275
CPH	R E CARBIDES	ANON	57	601601
CRYS	R E CARBIDES	ANON	57	601601
CRYS	R E CARBIDES	VICKERY R	58	601532
CRYS	R E CARBIDES	KLEBER, E	60	601450
CRYS	R E. CARBIDES	PALENIK, G	60	200914
CRYS	R E CARBIDES	SAMSONOV, G ZHURAV	60	600788
DF	R E. CARBIDES	MCCABE, C L	60	700599
ERES	R E CARBIDES	KLEBER, E	60	601450
MPP	R E. CARBIDES	GAUME MAHN, F	56	601048
MPP	R.E CARBIDES	SAMSONOV, G ZHURAV	60	600788
PHAS	R E CARBIDES	KLEBER E	60	601450
REAC	R E CARBIDES	KLEBER E	60	601450
REV	R E CARBIDES	KLEBER, E	60	601450
REV	R E CARBIDES	GAUME MAHN, F	56	601048
SPK	R E ELEMENTS	DIEKE, G CROSSWHIT	61	601406
SPK	R E ELEMENTS	ELYASHEVICH, M	53	601413
SPK	R E IONS	JUDD, B	56	601027
CRYS	R E IONS	JUDD, B	56	601027
BIB	R E METALS	KLEBER, E	60	601450
BIB	R E. METALS	SACHS, F	61	201059
CEMP	R E METALS	HSIPEH-LIN, S	61	200972
CPH	R.E METALS	MCKEOWN, J	58	601080
CRYS	R.E. METALS	KLEBER, E	60	601450
CRYS	R.E METALS	LADD, M LEE, W	61	601470
CRYS	R.E METALS	SAVITSKII, E TEREK	59	201067

CRYS	R.E. METALS	BANISTER, J LEGVOL	53	600674
CTEX	R.E. METALS	BARSON, F	57	601318
CTEX	R.E. METALS	BARSON, F LEGVOLD	57	601052
CTEX	R.E. METALS	CHANDRASEKHAR, B	58	601098
CTEX	R.E. METALS	BARSON, F	56	601499
CTEX	R.E. METALS	SPEDDING, F HANAK	61	201087
CTEX	R.E. METALS	BARSON, F LEGVOLD	53	601006
DH	R.E. METALS	SPEDDING, F EBERTS	59	601146
ERES	R.E. METALS	KLEBER, E	60	601450
MPP	R.E. METALS	SAVITSKII, E TEREK	59	201067
PHAS	R.E. METALS	LADD, M LEE, W	61	601470
PHAS	R.E. METALS	KLEBER, E	60	601450
REAC	R E. METALS	KLEBER, E	60	601450
REV	R.E METALS	SAVITSKII, E	61	201205
REV	R.E. METALS	KLEBER, E	60	601450
REV	R.E. METALS	AVGUSTINIK, A	63	301401
REV	R.E METALS	SACHS, F	61	201059
SPK	R.E METALS	PRANDTL, W	49	601408
SPK	R.E. METALS	ANON	59	601362
SPK	R E. METALS	BURBRIDGE, E	57	601103
THER	R E. METALS	MCKEOWN, J	58	601080
VAP	R.E. METALS	ANON	58	601524
VAP	R.E METALS	ANON	57	601308
CRYS	R E METALS	WARSHAW, I	61	201156
PHAS	R.E. METALS	WARSHAW, I	61	201156
MPP	R E. NITRIDES	GAUME-MAHN, F	56	601048
MPP	R.E. NITRIDES	LAVALLE, D	62	301517
MPP	R.E. NITRIDES	NACHMAN, J LUNDIN	62	301539
REV	R.E NITRIDES	GAUME-MAHN, F	56	601048
BIB	R.E OXIDES	KLEBER, E	60	601450
CPL	R.E. OXIDES	WESTRUM, E JUSTICE	62	601454
CPL	R.E. OXIDES	JUSTICE, B	61	601421
CRYS	R.E OXIDES	KLEBER, E	60	601450
CRYS	R.E. OXIDES	JUSTICE, B	61	601421
CRYS	R.E. OXIDES	MOZZI, R GUENTERT	62	300803
CTEX	R.E. OXIDES	STECURA, S CAMPBEL	61	201271
CTEX	R.E. OXIDES	BROWN, W KIRCHNER	61	601430
ERES	R.E. OXIDES	HARTMANN, W	36	601519
ERES	• R.E. OXIDES	NODDACK, W WALCH	59	601124
ERES	R.E. OXIDES	KLEBER, E	60	601450
ERES	R.E. OXIDES	NODDACK, I WALCH,H	59	601152
MISC	R.E. OXIDES	WESTRUM, E	60	600675
MSP	R.E. OXIDES	PANISH, M	61	601409
PHAS	R.E. OXIDES	COLLONGUES, R	61	201212
PHAS	R.E. OXIDES	WESTBROOK, J CARTE	61	601449
PHAS	R.E. OXIDES	BONDAR, I	60	200937
PHAS	R.E. OXIDES	KLEBER, E	60	601450
PHAS	R.E OXIDES	BRAUER, G GRADINGE	54	600978
REAC	R.E. OXIDES	KLEBER, E	60	601450
REV	R.E. OXIDES	KLEBER, E	60	601450
THER	R.E. OXIDES	JUSTICE, B	61	601421
THER	R.E. OXIDES	WHITE, D WALSH, P	62	601612
THER	R E OXIDES	WESTRUM, E JUSTICE	62	601454
THER	R.E. OXIDES	WHITE, D	60	601377
THER	R E OXIDES	WESTRUM, E	60	600675
THER	R E OXIDES	BREWER, L	52	601244
TRT	R E OXIDES	WARSHAW, I ROY, R	61	201358
VAP	R E OXIDES	WHITE, D WALSH, P	62	601612
VAP	R E OXIDES	HASAPIS, A MELVEGE	61	701039
VAP	R E OXIDES	KULVARSKAYA, B MAS	60	300399
VAP	R E OXIDES	SHCHUKAREV, S SEME	61	300653
VAP	R E OXIDES	WHITE, D	60	601377
VAP	R E OXIDES	PANISH, M	61	601409
VAP	R.E OXIDES	WALSH, P N GOLDSTE	60	700566
MPP	RE	ZEIDLER, E KRAUT	62	301627
MPP	RE	KOPETSKIY, CH	62	301270
MPP	RE	SAVITSKII, E	62	301344
ERES	RE	PIPPIG, E	61	201599
BIB	RE	WOHLL, M	60	700723
COPT	RE	BATSANOUA, L GRIGO	62	201752
CPH	RE	FINCH, R	61	700547
CPH	RE	BLANPAIN, R	61	300349
CPH	RE	TAYLOR, R	61	201250
CPL	RE	FINCH, R	61	700547
CPL	RE	BLANPAIN, R	61	300652
CPL	RE	TAYLOR, R	61	201250
CRYS	RE	LAWLEY, A	60	200801
CRYS	RE	FRANTSEVICH, I SHI	62	300513

MPP	REFRACTORY METALS	BESSERER, C	58	700929
PHAS	REFRACTORY METALS	MURPHY, A KENNEDY	60	701041
PMCH	REFRACTORY METALS	MURPHY, A KENNEDY	60	701041
REV	REFRACTORY METALS	MURPHY, A KENNEDY	60	701041
REV	REFRACTORY METALS	NORTHCOTT, L	61	700582
TCON	REFRACTORY METALS	BESSERER, C	58	700929
PHAS	RE TA SYST	KAUFMANN, A R RAPPR	61	300218
PHAS	RE V SYST	TYLKINA, M POVAROV	60	200935
PHAS	RE W C SYST	HAVELL, R BASKIN	61	201235
VAP	RE X	SHIMAZAKI, E NIWA	62	201503
VAP	RE X	MALM, J SELIG, H	61	201502
CEMP	RH	WHITE, G WOODS, S	57	601050
CPH	RH	DOUGLASS, R HOLDEN	59	700375
CPH	RH	JAEGER, F	31	900139
CPL	RH	JOHNSON, R HUDSON	56	601039
CPL	RH	BORELIUS, G	60	601168
CRYS	RH	BALE, E	58	601083
CRYS	RH	MCCALDIN, J DUWEZ	54	600956
CRYS	RH	THOMPSON, J	62	201648
DH	RH	PANISH, M REIF, L	61	700639
DH	RH	HAMPSON, R WALKER	61	700681
ERES	RH	CHASTON, J	62	300577
ERES	RH	PRICE, E TAYLOR, B	62	601473
ERES	RH	BRIDGMAN, P	51	400533
ERES	RH	KEMP, W KLEMENS, P	59	601205
MPP	RH	EREMENKO, V NAIDIC	61	300529
MPP	RH	FRANCIS, A	62	301076
PHAS	RH	MENDENHALL, C INGE	07	900143
PHAS	RH	ROESER, W WENSEL	34	900141
PHAS	RH	RAUB, E BEESKOW, H	59	201473
REV	RH	SANDERSON, L	61	300377
SPK	RH	MURPHY, R	52	600946
SPK	RH	SANCHO, F	58	601092
SPK	RH	SHADMI, Y	61	700954
SPK	RH	SANCHO, F	58	601091
SPK	RH	MOORE, C	58	601088
SPK	RH	NORRIS, J	60	601194
SPK	RH	CATALAN, M RICO, F	57	601206
TCON	RH	WHITE, G WOODS, S	57	601050
TCON	RH	POWELL, R TYE, R	56	601082
THER	RH	SCHICK, H ANTHROP	62	300995
THER	RH	KEMP, W KLEMENS, P	59	601205
REV	RH	BETTERIDGE, W RHYS	62	202003
THER	RH	DOUGLASS, R HOLDEN	59	700375
TRT	RH	ORIANI, R JONES, T	54	600954
TRT	RH	MCCALDIN, J DUWEZ	54	600956
TRT	RH	ROESER, W WENSEL	34	900141
TRT	RH	MENDENHALL, C INGE	07	900143
VAP	RH	DREGER, L	62	300720
VAP	RH	DREGER, L MARGRAVE	61	201500
VAP	RH	HASAPIS, A PANISH	60	700994
VAP	RH	BABELIOWSKY, T	62	300858
VAP	RH	DREGER, L	61	300528
VAP	RH	DREGER, L MARGRAVE	60	600643
VAP	RH	PANISH, M REIF, L	61	700639
VAP	RH	HAMPSON, R WALKER	61	700681
CRYS	RH B SYST	ARONSON, B ASELIUS	59	601166
VAP	RH CL SYST	BELL, W TAGAMI, M	62	201476
CPH	RH O	WOHLER, L JOCHUM	33	900124
DH	RH O	WOHLER, L JOCHUM	33	900124
DH	RH O	WOHLER, L MULLER	25	900140
THER	RH O	SCHICK, H ANTHROP	62	300995
THER	RH O 2	ALCOCK, C HOOPER	60	601161
CPH	RH2O	WOHLER, L JOCHUM	33	900124
DH	RH2O	WOHLER, L JOCHUM	33	900124
DH	RH2O	WOHLER, L MULLER	25	900140
CPH	RH2O 3	WOHLER, L JOCHUM	33	900124
DH	RH2O 3	WOHLER, L JOCHUM	33	900124
DH	RH2O 3	WOHLER, L MULLER	25	900140
THER	ROCKET ENGINES	NIKOLAYEV, B	60	400615
COPT	RU	DOUGLAS, R W ADKIN	61	700614
CRYS	RU	LAWLEY, A	60	200801
CRYS	RU	MCCALDIN, J DUWEZ	54	600956
CRYS	RU	THOMPSON, J	62	201648
MPP	RU	FRANCIS, A	62	301076
PHAS	RU	DOUGLAS, R W ADKIN	61	700614
SPK	RU	TREES, R	61	701067
SPK	RU	SHADMI, Y	61	700954

SPK	RU		
MOORE, C		58	601088
THER	RU		
MARGRAVE, J		61	700967
THER	RU		
ZOUBOV, N POURBAIX		58	601076
TRT	RU		
MCCALDIN, J DUWEZ		54	600966
VAP	RU		
PAULE, R		61	601479
VAP	RU		
HASAPIS, A MELVEGE		61	701039
VAP	RU		
MARGRAVE, J		61	700967
VAP	RU		
PANISH, M REIF, L		62	300721
CRYS	RU B SYST		
KEMPTER, C FRIES		61	701050
CRYS	RU B SYST		
ARONSON, B STENBER		62	300757
CRYS	RU B SYST		
KEMPTER, C FRIES		61	201103
MPP	RU B SYST		
BUDDERY, J WELCH		51	600940
PHAS	RU B SYST		
ROOF, R KEMPTER, C		62	300966
PHAS	RU B SYST		
OBROWSKI, W		63	301545
CRYS	RU C		
KEMPTER, C NADLER		60	701010
CRYS	RU C		
KEMPTER, C NADLER		60	201024
CRYS	RU C		
KEMPTER, C NADLER		60	201024
PHAS	RU C		
NADLER, M KEMPTER		60	300301
THER	RU O		
ALCOCK, C HOOPER		60	601161
DH	RU O 2		
SCHNEIDEREITTI, G		62	301582
DH	RU O 2		
SCHAEFER, H SCHNEI		63	301577
SPK	RU O 4		
ORTNER, N ANDERSON		59	701066
THER	RU O 4		
ORTNER, N ANDERSON		59	701066
THER	RU O 4		
ZOUBOV, N POURBAIX		58	601076
TRT	RU O 4		
NIKOLSKII		63	301541
THER	RU OXIDES		
ORTNER, N ANDERSON		59	701066
VAP	RU OXIDES		
ORTNER, N ANDERSON		59	701066
PHAS	RU RE		
RUDY, E KIEFFER, B		62	201556
PHAS	RU RE		
SAVITSKII, E TYLKI		62	201531
PHAS	RU TA SYST		
KAUFMANN A R RAPPR		61	300218
PHAS	RU W SYST		
KAUFMANN A R RAPPR		61	300218

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VAP	SC		
KRIKORIAN, O		63	301284
CEMP	SC		
MICHAELSON, H		50	400529
CPH	SC		
MARDON, P NICHOLS		61	701025
CPL	SC		
MONTGOMERY, H PELL		61	601447
CPL	SC		
LEBEDEV, V		48	700702
CPL	SC		
WELLER, W KELLEY		62	700704
CRYS	SC		
MARDON, P NICHOLS		61	701025
CRYS	SC		
SPEDDING, F DAANE		56	700703
CRYS	SC		
HERRMANN, K DAANE		55	700905
ERES	SC		
COLVIN, R ARAJS, S		63	301036
ERES	SC		
MARDON, P NICHOLS		61	701025
MPP	SC		
MARDON, P NICHOLS		61	200987
MPP	SC		
SPITSYN, V KOMISSA		61	300370
MPP	SC		
BORISENKO, L		61	300447
MPP	SC		
SPEDDING, F DAANE		60	700713
MPP	SC		
HILLER, M		60	700738
PHAS	SC		
BEAUDRY, B DAANE		62	300573
PHAS	SC		
FISCHER, W BRIINGE		37	700765
REAC	SC		
SPITSYN, V KOMISSA		61	300370
REV	SC		
SANDERSON, L		61	300376
REV	SC		
STRUAT K WEIK, H		60	601167
REV	SC		
VICKERY, R		60	601173
REV	SC		
LOVE, B		60	700735
REV	SC		
GEISELMAN, D		62	201941
SPK	SC		
ROSENZWEIG, N PORT		60	700996
SPK	SC		
MERRILL, P GREENST		56	601007
SPK	SC		
GARSTANG, R		52	100207
SPK	SC		
WRIGHT, K		48	100212
SPK	SC		
SKINNER, H		55	700761
SPK	SC		
ROSENZWEIG, N PORT		60	700901
THEO	SC		
ROSENZWEIG, N PORT		60	700996
THEO	SC		
ROSENZWEIG, N PORT		60	700901
TRT	SC		
BEAUDRY, B DAANE		62	300573
TRT	SC		
FISCHER, W BRIINGE		37	700765
VAP	SC		
KARELIN, V NESMEYA		62	300362
VAP	SC		
BEAVIS, L		60	600659
VAP	SC		
ACKERMANN, R RAUH		62	700840
VAP	SC		
KARELIN, V NESMEYA		62	601594
VAP	SC		
BEAVIS, L		60	701016
VAP	SC		
ACKERMANN, J RAUH		62	700909
THER	SC +		
VASILEV, V ZOLOTAR		59	700823
CEMP	SC B 2		
KUDINTSEVA, G NESH		62	301514
CEMP	SC B 2		
SAMSONOV, G FOMENK		63	202128
CRYS	SC B 2		
ZHURAVLEV, N STEPA		58	700727

MPP	SC B 2	SAMSONOV, G	61	700728
TRT	SC B 2	SAMSONOV, G	61	700728
PHAS	SC B 6	PRZYLYLSKA, M REDD	63	300962
PHAS	SC BE13	LAUBE, E NOWOTNY	62	201750
SURF	SC BORIDES	FOMENKO, V	61	201420
MISC	SC C	NOWOTNY, H ABER-WE	61	700651
MISC	SC C	SAMSONOV, G MAKAVE	62	700744
PHAS	SC C	AVER-WELSBACH, H	61	201175
CRYS	SC F 3	AKISHIN, P NAURMOV	61	201201
SPK	SC F 3	AKISHIN, P NAURMOV	61	201201
THER	SC ION	VASILEV, V ZOLOTAR	59	700823
MPP	SC N	FRIEDERICH, E SITT	25	700766
REAC	SC N	LYUTAYA, M BUKHANE	62	301528
CRYS	SC O	VICKERY, R SEDALEK	59	700707
F	SC O	BREWER, L CHARDRAS	59	700721
REAC	SC O	MASSONNE, J	61	201425
SPK	SC O	AKERLIND, L	62	300611
SPK	SC O	AKERLIND, L	61	700635
SPK	SC O	BERG, R SIMANOGLN	60	301089
DH	SC2O 3	HUBER, E FITZGIBBO	63	301246
DH	SC2O 3	HUBER, E FITZGIBBO	63	202057
CEMP	SC2O 3	MORIN, F	58	700710
CPL	SC2O 3	WELLER, W KING, E	63	301617
CRYS	SC2O 3	MILLIGAN, W VERNON	53	700756
DH	SC2O 3	HUBER, E HOLLEY, C	62	700704
DH	SC2O 3	MAH, A	62	700705
PHAS	SC2O 3	BARTA, C PETRU, F	58	700725
REAC	SC2O 3	SPEDDING, F POVELL	58	700757
THER	SC2O 3	KUBASHEVSKI, O EVA	56	700829
TRT	SC2O 3	BARTA, C PETRU, F	58	700725
THEO	SEMICONDUCTORS	HARVEY, W	63	202047
BIS	SI	SULLIVAN, R SEIBEL	60	701038
CEMP	SI	SAMSONOV, G NESHPO	59	201052
COPT	SI	GOLDSMITH, A HIRSC	60	700930
CPH	SI	GOLDSMITH, A HIRSC	60	700930
CPH	SI	KANTOR, P KISIL, O	60	300274
VAP	SI	DROWART, J DEMARIA	59	301212
CPH	SI	SHARAN, B SINGH, S	60	600654
CPH	SI	WILLIAMS, N N	61	700659
CPL	SI	KEESOM, P H PEARLM	52	300170
CPL	SI	PEARLMAN, N KEESOM	52	300171
CPL	SI	FLUBACHER, P LEADB	59	300391
CPL	SI	SHARAN, B SINGH, S	60	600654
CRYS	SI	GETTE, E FOOTE, F	35	700510
DHT	SI	DAVIS, S ANTHROP	61	701009
ERES	SI	GOLDSMITH, A HIRSC	60	700930
H	SI	GOLDSMITH, A HIRSC	60	700930
KIN	SI	CHAPMAN, A	60	200810
MSP	SI	KOYLOVSKAYA, V		301103
MSP	SI	LOWRIE, R	60	701014
PHAS	SI	BEREZHNOI, A KORDY	62	201553
PHAS	SI	GELD, P GERTMAN, Y	60	300417
REV	SI	BEREZHNOI, A	61	201469
SPK	SI	ELYASHEVICH, M NIK	56	301090
SPK	SI	SHENSTONE, A	61	700636
SPK	SI	NIKITINA, O	61	200818
SPK	SI	HOLMES, J HOOVER	62	300822
TCON	SI	GOLDSMITH, A HIRSC	60	700930
TCON	SI	HOLLAND, M	61	201289
THER	SI	CHERKASKIN, Y GLAD	57	301107
THER	SI	SCHICK, H ANTHROP	63	300994
THER	SI	SULLIVAN, R SEIBEL	60	701038
THER	SI	WILLIAMS, N N	61	700659
TRT	SI	WENTORF, R KASPER	63	301620
TRT	SI	KANTOR, P KISIL, O	60	300274
VAP	SI	KOSENKO, V NESTERE	61	600847
VAP	SI	ROTH, E MARGERUM	62	300970
VAP	SI	POPPER, P	60	601632
VAP	SI	LOWRIE, R	60	701014
VAP	SI	DAVIS, S ANTHROP	61	701009
VAP	SI	HANLIN, H	60	700951
CRYS	SI	JAMIESON, J	63	202062
VAP	SI	ZADUMKIN, S	59	300284
VAP	SI	TSEPLYAEVA, A PRIS	60	300400
SPK	SI+++	TORESSON, Y	60	200804
SPK	SI2	VERMA, R WARSOP, P	63	301032
REAC	SI B 4	FEIGELSEN	62	301446
REAC	SI B 6	FEIGELSEN	62	301446

MPP	SI B SYST	WEBER, B RIZZO, H	63	202159
PHAS	SI B SYST	SAMSONOV, G SLEPTS	62	301341
PHAS	SI B SYST	ANON	60	701015
VAP	SI B SYST	ANON	60	701015
REAC	SI B SYST	BROSSET, C MAGNUSS	60	200932
MPP	SI B SYST	NOETH, H HOELLERER	62	301542
BIB	SI B SYST	SULLIVAN, R SEIBEL	60	701038
THER	SI B SYST	SULLIVAN, R SEIBEL	60	701038
KIN	SI B SYST	WILLIAMS, E	61	300260
PHAS	SI B C SYST	KALINIAN, A SHAMRA	60	301267
VAP	SI C	DROWART, J DEMARIA	59	301212
VAP	SI C	FESENKO, V BOLGAR	63	301216
CEMP	SI C	HORI, J	62	301478
CRYS	SI C	KNIPPENBERG, W HAS	62	301265
CRYS	SI C	KRISHNA, P VERMA	63	301287
DF	SI C	REIN, R CHIPMAN, J	63	301327
DHD	SI C	STEELE, W NICHOLS	62	301596
MPP	SI C	KAMAMURA, T HAYASH	62	301492
REV	SI C	DOBROLEZH, S ZUBKO	63	301437
TCON	SI C	BOSCH, G	61	201505
COPT	SI C	BRESKER, R VORONIN	59	300799
CRYS	SI C	TOMITA, T	60	600801
REV	SI C	BROWN, A	60	701044
TRT	SI C	WHITNEY, E	63	202160
CRYS	SI C	MERZ, K ADAMSKY, R	60	202103
VAP	SI C	HONIG, R	62	202055
MPP	SI C	KIRCHNER, H KNOLL	63	202069
CRYS	SI C	KRISHNA, P VERMA	63	202084
CRYS	SI C	BAUER, J FIALA, J	63	201998
REV	SI C	CHADWICK, U	63	202015
DH	SI C	DAVIS, S ANTHROP	61	701009
DHT	SI C	DAVIS, S ANTHROP	61	701009
VAP	SI C	DAVIS, S ANTHROP	61	701009
DH	SI C	DENTREMONT, J CHIP	63	300841
REAC	SI C	POCH, W DIETZEL, A	62	202119
REAC	SI C	DIETZEL, H JAGODZI	60	700676
THER	SI C	DIETZEL, H JAGODZI	60	700676
DH	SI C	DROWART, J DEMARIA	60	200770
THER	SI C	DROWART, J DEMARIA	60	200770
VAP	SI C	DROWART, J DEMARIA	60	200770
THER	SI C	GRIEVESON, P ALEOC	60	301060
CRYS	SI C	JAGODZINSKI, H ARN	60	200898
KIN	SI C	JORGENSEN, P	60	200924
KIN	SI C	JORGENSON, P WADSW	60	200772
DF	SI C	KIRKWOOD, D K CHIP	61	700634
CRYS	SI C	KRISHNA, P VERMA	61	701058
SPK	SI C	OVCHARENKO, I TUNI	60	600778
THER	SI C	POPPER, P	60	601632
COPT	SI C	SAMSONOV, G PENKOV	61	300800
CPL	SI C	SHMIDT, N SOKOLOV	60	201590
DF	SI C	SMILTENS, J	60	301059
DH	SI C	SMILTENS, J	60	200771
THER	SI C	SMILTENS, J	60	200771
VAP	SI C	SMILTENS, J	60	200771
ZKP	SI C	SMILTENS, J	60	200771
BIB	SI C	SULLIVAN, R SEIBEL	60	701038
THER	SI C	SULLIVAN, R SEIBEL	60	701038
CRYS	SI C	TAYLOR, A JONES, R	60	200776
CTEX	SI C	TAYLOR, A JONES, R	60	200776
CRYS	SI C	TOMITA, T	60	600801
THEO	SI C	TSERTSVADZE, A TCH	62	300583
SPK	SI C	VIDALE, G	60	201616
VAP	SI C	VIDALE, G	60	201616
MPP	SI C	VORONIN, N	61	301007
CPH	SI C	WALKER, [illegible] EWING, C	62	301098
PHAS	SI C	YASUDA, S	62	300581
THER	SI CARBIDES	SAMSONOV, G	59	201343
DH	SI CARBIDES	DROEGE, J	60	201160
PHAS	SI C SYST	SEARCY, A FINNE, L	62	201874
PHAS	SI C SYST	DOLLOFF, R	60	700989
PHAS	SI C SYST	DOLLOFF, R	60	600662
REAC	SI C SYST	KUHN, W	63	300919
DH	SI C SYST	SCACE, R SLACK, G	60	200768
PHAS	SI C SYST	SCACE, R SLACK, G	60	200768
PHAS	SI C O SYST	KRIVSKY, W SCHUMAN	61	300459
MPP	SILICATES	LIPMAN, R	59	400596
MPP	SILICIDES	SAMSONOV, G	59	202126
CRYS	SILICIDES	NESHPOR, V SAMSONO	62	202108

CRYS	SILICIDES	LUNDIN, C	61	202089
CPH	SILICIDES	GELD, P KRENTSIS	63	202037
CRYS	SILICIDES	GLADYSHEVSKII, E	63	202040
CRYS	SILICIDES	NESHPOR, V	61	300792
DH	SILICIDES	GOLUTVIN, Y	62	300567
MPP	SILICIDES	SAMSONOV, G	59	400619
PHAS	SILICIDES	PORTNOY, K	60	700944
REV	SILICIDES	SAMSONOV, G	62	300989
CRYS	SILICIDES-PT MET	ARONSSON, B RUNDQV	61	300504
CRYS	SI N	BORGEN, O SEIP, H	61	201514
SPK	SI N	STEVENS, A FERGUSO	63	202143
REAC	SI N	HENGGE, E	62	201759
VAP	SI3N 4	FESENKO, V BOLGAR	63	301216
REV	SI3N 4	RABENAU, A	63	301324
CTEX	SI3N 4	IWAI, S YASUNAGA	59	700684
THER	SI NITRIDES	SAMSONOV, G	59	201343
ERES	SI N SYST	SAMSONOV, G	61	601585
PHAS	SI N SYST	SAMSONOV, G	61	601585
DF	SI O	WHATLEY, L	62	201679
DH	SI O	BERGMAN, G MEDVEDE	59	300674
DH	SI O	BERGMAN, G MEDVEDE	59	300674
MPP	SI O	YORK, D	63	301019
PHAS	SI O	BREWER, L MASTIK	49	601634
PHAS	SI O	BRCIC, B GOLIC, L	62	201636
PHAS	SI O	CHAPMAN, A ST PIER	60	301427
REAC	SI O	EMONS, H BOENICKE	62	300562
REAC	SI O	WHITE, P	62	300732
SPK	SI O	NICHOLLS, R	62	601625
SPK	SI O	NICHOLLS, R	62	300698
SPK	SI O	MCGREGOR, A NICHOL	61	300476
SPK	SI O	JAMES, T	63	301481
SPK	SI O	JAMES, T	63	301252
SPK	SI O	BARROW, R ROWLINSO	54	600896
SPK	SI O	ROWLINSON, N	53	600916
SPK	SI O	VERMA, R MULLIKEN	61	700637
THER	SI O	RAMSTAD, H F RICHA	61	300188
THER	SI O	RAMSTAD, H RICHARD	61	300339
THER	SI O	SCHICK, H ANTHROP	63	301579
THER	SI O	RAMSTAD, H RICHARD	61	300458
CPL	SI O 2	WESTRUM, E	60	701021
CRYS	SI O 2	SCLAR, C CARRISON	62	301584
CRYS	SI O 2	FLOERKE, O	62	301449
CRYS	SI O 2	ANIKINA, L	62	301173
CRYS	SI O 2	ARNOLD, H	62	301175
MPP	SI O 2	NAGARJAN, G	63	202106
REAC	SI O 2	LEONOV	61	301522
SPK	SI O 2	SODA, R	62	301591
THER	SI O 2	SCHICK, H ANTHROP	63	301580
THER	SI O 2	SCHICK, H	60	202130
CRYS	SI O 2	SMITH, G ALEXANDER	63	202139
CRYS	SI O 2	SMITH, G	63	202140
MPP	SI O 2	STEPIN, B	63	202142
REAC	SI O 2	KAY, D TAYLOR, J	63	202066
REAC	SI O 2	KOMATSU, N GRANT	62	202077
PHAS	SI O 2	BEREZNOI, A GULKO	61	202002
TRT	SI O 2	SCLAR, C CARRISON	62	301585
TRT	SI O 2	CHAKLADER, A	63	301425
TRT	SI O 2	CHAKLADER, A	63	301426
TRT	SI O 2	CHAKLADER, A	63	301201
PHAS	SI O 2	DACHILLE, F ROY, R	59	301210
CPH	SI O 2	MITKINA, E	60	301306
TRT	SI O 2	SEMENCHENKO, V	61	301349
CRYS	SI O 2	STISHOV, S BELOV	62	301363
DH	SI O 2	WISE, S MARGRAVE	63	301381
CPL	SI O 2	CLARK, A STRAKNA	62	300580
CRYS	SI O 2	EMONS, H BOENICKE	62	300562
CRYS	SI O 2	HOLMQUIST, S B	61	700517
CRYS	SI O 2	PREISINGER, A	62	300963
CRYS	SI O 2	TROMEL, G KRISEMEN	59	700690
CRYS	SI O 2	STISHOV, S POPOVA	61	201716
DH	SI O 2	WISE, S	62	300741
DH	SI O 2	GOOD, W	62	300394
DH	SI O 2	COCHRAN, C FOSTER	62	300395
DH	SI O 2	WISE, S MARGRASE	62	300396
DHT	SI O 2	MACKENZIE, J D	60	300139
EMF	SI O 2	BENZ, R WAGNER, C	61	700640
F	SI O 2	CHIPMAN, J	61	201050
KIN	SI O 2	AINSLIE, N MACKENZ	61	600837

MPP	SI O 2		
GREBENSHCHIKOV, R		60	200973
PHAS	SI O 2		
GIELISSE, P		62	201740
PHAS	SI O 2		
ARAMAKI, S ROY, R		62	201695
PHAS	SI O 2		
TROMEL, G KRISEMEN		59	700690
PHAS	SI O 2		
MORIYA, Y			201363
PHAS	SI O 2		
KHLAPOVA, A		62	301146
PHAS	SI O 2		
KHLAPOVA, A		61	201848
PHAS	SI O 2		
TOROPOV, N GALAKHO		61	201965
REAC	SI O 2		
KAY, D TAYLOR, J		60	300131
SPK	SI O 2		
MARKIN, E SOBOLEV		60	200979
SPK	SI O 2		
SODA, R		61	201302
TCON	SI O 2		
WRAY, K CONNOLLY		59	600620
THER	SI O 2		
KAY, D TAYLER, J		60	300131
TRT	SI O 2		
BOYD, F ENGLABD, J		63	301193
THER	SI O 2		
MACKENZIE, J D		60	300139
THER	SI O 2		
RAMSTAD, H RICHARD		61	300339
VAP	SI O 2		
NESMEYANOV, A FIRS		60	200953
VAP	SI O 2		
FIRSOVA, L NESMEYA		60	701004
VAP	SI O 2		
FIRSOVA L NESEMEY		60	200761
PHAS	SI2O 3		
DADAPE, V MARGRAVE		62	300551
PHAS	SI2O 3		
CREMER, E FAESSLER		59	201034
SURF	SI OXIDES		
LEPINSKIKH, B		60	201215
VAP	SI OXIDES		
FIRSOVA, L NESMEYA		60	201020
VAP	SI OXIDES		
NESMEYANOV, A FIRS		59	201019
PHAS	SI O SYST		
FLOERKE, O		61	301220
MPP	SI O SYST		
APPEN, A KAIALOVA		62	300589
THEO	SI O SYST		
VORONKOV, M		61	301004
CPH	SI V SYST		
GOLUTVIN, Y KOZLOV		62	300568
SPK	SIMPLE MOLECULES		
DOUGLAS, A		55	600678
CPH	SM		
ARAJS, S COLVIN, R		62	300751
CPH	SM		
JENNINGS, L HILL		59	601197
CPL	SM		
DREYFUS, B GOODMAN		61	601417
CPL	SM		
ROBERTS, L		57	601089
CPL	SM		
LOUNASMAA, O		62	300780
CRYS	SM		
DAANE, A RUNDLE, R		53	601215
CRYS	SM		
DAANE, A RUNDLE, R		54	601230
CRYS	SM		
ELLINGER, F ZACHAR		53	600947
DH	SM		
HUBER, E		55	601272
DH	SM		
HUBER, E MATTHEWS		55	601008
DH	SM		
SAVAGE, W HUDSON		59	601126
ERES	SM		
OLSEN, C		60	601336
ERES	SM		
ALSTAD, J COLVIN		61	201099
SPK	SM		
DREYFUS, B GOODMAN		61	601417
SPK	SM		
SCHWARZSCHILD, M		57	601047
SPK	SM		
BURBRIDGE, E BURBR		55	601003
SPK	SM		
SMITH, K SPALDING		62	300777
SPK	SM		
GARSTANG, R		52	100207
SPK	SM		
MCNALLY, J		52	100211
SPK	SM		
SMITH, D MCNALLY		50	100197
SPK	SM		
BRIX, P		49	400527
SPK	SM		
BRIX, P KOPFERMANN		49	400543
SPK	SM		
GRATTON, L		52	400567
SPK	SM		
BRIX, P KOPPERMAN		52	400574
SPK	SM		
BODMER, A		54	600936
SPK	SM		
STRIGANOV, A KATUL		62	601468
SPK	SM		
MURAKAWA, K		54	600958
SPK	SM		
DIEKE, G SARUP, R		62	201718
SPK	SM		
FEDOFILOV, P KAPLY		62	201755
THER	SM		
SPEDDING, F H MCKE		60	700570
TRT	SM		
ANON		53	601502
VAP	SM		
ANON		56	601319
VAP	SM		
SAVAGE, W HUDSON		59	601126
PHAS	SM B 4		
GALLOWAY, G		62	701078
REAC	SM B 4		
GALLOWAY, G		62	701078
CEMP	SM B 6		
SAMSONOV, G PADERN		59	300143
ERES	SM B 6		
PADERNO, Y SAMSONO		61	301072
PHAS	SM B 6		
GALLOWAY, G		62	701078
REAC	SM B 6		
SAMSONOV, G ZHURAV		59	201758
CRYS	SM B SYST		
ANON		61	601376
CRYS	SM N		
EICK, H BAENZIGER		56	601046
ERES	SM N		
DIDCHENKO, R GORTS		63	301435
PHAS	SM N		
EICK, H BAENZIGER		56	601046
REAC	SM N		
EICK, H BAENZIGER		56	601046
REAC	SM NITRIDES		
EICK, H		57	601053
CRYS	SM O		
ELLINGER, F ZACHAR		53	600947
VAP	SM O		
KULVARSHAYA, B MAS		60	301064
SPK	SM2		
BURBRIDGE, G BURBR		54	600937
CPH	SM2O 3		
PANKRATZ, L KING		62	300958

CPL	SM2O 3		
JUSTICE, B WESTRUM		63	300907
CRYS	SM2O 3		
STARITZKY, E		56	601257
CRYS	SM2O 3		
KUTSEV, V SMAGINA		63	301515
CRYS	SM2O 3		
CROMER, D		57	601304
CRYS	SM2O 3		
CROMER, D		57	601062
CRYS	SM2O 3		
DOUGLASS, R STARIT		56	601011
CTEX	SM2O 3		
PLOETZ, G		57	601309
MSP	SM2O 3		
PANISH, M		61	601372
TRT	SM20 3		
WISNYI, L PIJANOWS		57	601056
VAP	SM2O 3		
PANISH, M		61	601372
PHAS	SM OXIDES		
EICK, H BAENZIGER		56	601070
REAC	SM OXIDES		
EICK, H BAENZIGER		56	601070
REAC	SM OXIDES		
EICK, H		57	601053
BIB	SN OXIDES		
JONES, P		60	200984
CRYS	SM O SYST		
EICK, H		56	601289
PHAS	SM O SYST		
EICK, H		56	601289
MPP	SOLAR FURNACE		
MANVELYAN, M MELIK		61	400606
THEO	SOLID STATE		
DEKHTYAR, I		59	300411
CEMP	SOLIDS		
KUCHEROV, R YA RIK		60	300154
CPH	SOLIDS		
IVANOVA, L I		61	300249
THER	SOLIDS		
GLUSHKO, V		62	301221
THEO	SOLIDS		
IVERONOVA, V ZOYAG		63	202061
THER	SOLIDS		
MARINCHUK, A MOSKA		63	202092
CPH	SOLIDS		
LANDIYA, N TSAGARE		62	301516
CPH	SOLIDS		
ROSENSTOCK, H		61	301563
CRYS	SOLIDS		
BRADLEY, J		63	301411
DH	SOLIDS		
VOROBEV, A PRIVA		60	300135
PHAS	SOLIDS		
SCHAFER, K		60	300133
PHAS	SOLIDS		
IVANOVA, L I		61	300249
PHAS	SOLIDS		
DEVRIES, K BAKER		60	600665
REAC	SOLIDS		
BUDNIKOV, P GINSTL		61	300315
REV	SOLIDS		
SWALIN, R		62	300703
THEO	SOLIDS		
SCHAFER, K		60	300133
THEO	SOLIDS		
ORMONT, B		63	301317
THEO	SOLIDS		
KRESTOVNIKOV, A VI		60	301512
THEO	SOLUBILITY		
WABER, J GSCHNEIDE		63	301374
THEO	SOLUTIONS		
KHACHATURYAN, A		63	202067
THER	SOLUTIONS		
KLEPPA, O		62	301503
THEO	SPECIFIC HEAT		
WAJTOWICZ, P J KIR		60	700641
THEO	SPECIFIC HEAT		
ROSENSTOCK, H B		61	700643
THEO	SPECTRA		
MASON, S		61	201224
THEO	SPECTROSCOPY		
GRIBOV, L		62	900220
THEO	SPECTROSCOPY		
VARSHNI, V P SHUKL		61	700698
BETA	SR		
EVDOKIMOVA, V VERE		60	201072
SPK	SR		
PENKIN, N SHABANOV		62	601601
SPK	SR		
CODLING, K		61	600775
SPK	SR		
SHADMI, Y		61	700954
VAP	SR		
KOZHEVNIKOV, G		63	301510
CEMP	SR B 6		
JOHNSON, R DAANE		63	301489
DH	SR B 6		
SAMSONOV, G SEREBR		61	601581
ERES	SR B 6		
SAMSONOV, G SEREBR		61	601581
THER	SR B 6		
BOLGAR, A		61	700938
VAP	SR B 6		
SAMSONOV, G SEREBR		61	601581
VAP	SR B 6		
BOLGAR, A		61	700938
CRYS	SR2MG17		
KRIPYAKEVICH, P			201670
PHAS	SR MG SI SYST		
DEAR, P		60	201548
DH	SR O		
MAH, A		63	202093
E	SR O		
LAGERQVIST, A HULD		54	600681
ERES	SR O		
ADAMS, M JACOB, L		60	200763
SPK	SR O		
LAGERQVIST, A ALMK		54	600680
SPK	SR O		
NICHOLLS, R		62	300698
SPK	SR O		
HULDT, L LAGERQVIS		55	600893
SPK	SR O		
HULDT, L LAGERQVIS		56	600894
SPK	SR O		
VEITS, I GURVICH		57	600899
SPK	SR O		
ALMQVIST, G LAGERQ		49	600922
THER	SR O		
SCHICK, H ANTHROP		62	300995
VAP	SR O		
METSON, G		63	301536
CEMP	SR OXIDES		
PALGUEV, S NECEIMI		62	201717
DHD	SR OXIDES		
VEITS, I GURVICH		56	700964
THER	SR OXIDES		
VEITS, I GURVICH		56	700964
THER	SR OXIDES		
ORTNER, N ANDERSON		59	701066
VAP	SR OXIDES		
ORTNER, N ANDERSON		59	701066
CPH	SUBSTANCES		
IVANOVA, L		61	201347
THER	SUBSTANCES		
OSBORN, D STEIN, L		62	201923
REV	SUBSTANCES		
OSBORN, D STEIN, L		62	201923
REAC	SULFABORIDES		
FLAHAUT, J DOMANGE		62	300512
SPK	SUN		
GOLDBERG, L MULLER		53	600710
VAP	SURFACES		
TSVETAEV, A GLAZUN		61	300768

THEO	SYSTEMS	NECKEL, A	61	300509

T

BOOK	TA	SAMSONOV, G KONSTA	61	301570
CPH	TA	JOHNSON, R	60	301488
CPL	TP	FEATHERSTON, F NEI	63	301444
MPP	TA	FRERICHS, R	62	301450
MPP	TA	KOPETSKIY, CH.	62	301270
CPH	TA	KRAFTMACHER, IA	62	301282
VAP	TA	CANO, G	62	301423
BETA	TA	KRUPNIKOU, K BAKAN	63	301149
BIB	TA	WENSRICH, C	60	700972
BIB	TA	ANON	60	701022
BIB	TA	WOHLL, M	60	700723
BIB	TA	WENSRICH, O	60	700890
CEMP	TA	RICKERT, E BECKETT	49	601638
CPH	TA	FINCH, R	61	700547
CPH	TA	RASOR, N MCCLELLAN	60	700896
CPH	TA	LEHMAN, G	60	300304
CPH	TA	CARTER, W	61	601631
CPH	TA	HOCH, M	61	201167
CPH	TA	RASOR, N MCCLELLAN	60	700984
CPH	TA	TAYLOR, R	61	201250
CPL	TA	FINCH, R	61	700547
CPH	TA	HOCH, M JOHNSTON	61	700613
CPL	TA	TAYLOR, R	61	201250
CPL	TA	BORELIUS, G	60	601168
CPL	TA	BOORSE, H BERMAN	56	700887
CPL	TA	COCHRAN, J	62	201877
CRYS	TA	VASUTINSKY, B KART	62	301009
CRYS	TA	EDWARDS, J SPEISER	51	601179
CRYS	TA	FERRISS, D ROSE, R	62	301137
CTEX	TA	EDWARDS, J SPEISER	51	601179
CTEX	TA	CARTER, W	61	601631
CTEX	TA	RASOR, N MCCLELLAN	60	700984
SPK	TA	CLAUS, H ULMER, K	63	202017
CTEX	TA	NOWOTNY, H LAUBE	61	600844
ELCH	TA	MONNIER, R GRANDJE	60	200949
ERES	TA	FINCH, R	61	700547
ERES	TA	BRIDGMAN, P	51	400533
ERES	TA	TYE, R	61	201117
ERES	TA	TAYLOR, R	61	201250
KIN	TA	KOFSTAD, P	61	201400
MISC	TA	HAMPEL, C	61	200889
MISC	TA	BASKIN, M TRETYAKO	62	201951
MPP	TA	RICKERT, E BECKETT	49	601638
MPP	TA	RASOR, N MCCLELLAN	60	700896
MPP	TA	ARGENT, B MILNE, G	60	201039
MPP	TA	RILEY, W MCCLELLAN	62	301080
MPP	TA	MYERS, R	50	500130
PHAS	TA	HAWORTH, C	60	201017
PHAS	TA	SHAFFER, P	61	700941
PHAS	TA	ERBEN, E LESSER, R	61	300323
PHAS	TA	ROSTOKER, W	60	201396
PHAS	TA	VASYUTINSKII, B	62	201776
PMCH	TA	BOLEF, D	61	200936
PREP	TA	MILLER, G	62	201943
REAC	TA	MILLER, G	60	200834
REAC	TA	DEUTSCH, N ERVIN	60	500123
REAC	TA	COWGILL, M STRINGE	60	500122
REAC	TA	FRANTSEVICH, I LAV	59	200869
REAC	TA	FAIRBROTHER, F COW	59	200886
REAC	TA	KUBASCHEWSKI, O HO	60	201036
REAC	TA	SCHAFER, H SIBBING	60	201085
REAC	TA	ENGELKE, J HALDEN	60	201529
REAC	TA	KONSTANTINOV, V	62	301146
REV	TA	BARTLETT, E SCHMID	61	701052
REV	TA	WOHLL, M	60	701053
REV	TA	ERBEN, E LESSER, R	61	300323
REV	TA	SYRE, R	61	201579
SPK	TA	ALLEN, R GLASIER	60	200828
SPK	TA	ROSENZWEIG, N PORT	60	700996
SPK	TA	TREES, R	61	701067
SPK	TA	ROSENZWEIG, N PORT	60	700901
SPK	TA	MOORE, C	58	601088
SPK	TA	KIESS, C	62	201678
TCON	TA	RASOR, N MCCLELLAN	60	700984

TCON	TA		
RASOR, N MCCLELLAN		60	700896
TCON	TA		
TYE, R		61	201117
TCON	TA		
CONNOLY, A MENDELS		62	201536
THEO	TA		
ROSENZWEIG, N PORT		60	700996
THEO	TA		
ROSENZWEIG, N PORT		60	700901
THER	TA		
SCHICK, H ANTHROP		63	300994
THER	TA		
CARTER, W		62	300749
THER	TA		
CARTER, W		61	601631
THER	TA		
RASOR, N MCCLELLAN		60	200960
TRT	TA		
WILLIAMS, D JACKSO		62	301016
TRT	TA		
MCMASTERS, O LARSE		61	600834
VAP	TA		
GEBHARDT, E SEGHEZ		62	601676
VAP	TA		
BABELIOWSKY, T		62	300858
KIN	TA SYST		
KUBASCHEWSKI, O		62	601577
THER	TA SYST		
KUBASCHEWSKI, O		62	601577
PHAS	TA AL C		
JEITSCHKO, W NOWOT		63	301485
THER	TA B		
LEITNAKER, J BOWMA		62	300553
THER	TA B		
MEERSON, G		60	300298
CEMP	TA B 2		
MATSKEVICH, T KRAC		62	301533
H	TA B 2		
MEZAKI, R TILLEUX		62	601617
MPP	TA B 2		
MALYUCHKOV, O POVI		62	202095
S	TA B 2		
MEZAKI, R TILLEUX		62	601617
CRYS	TA3B 2		
KIEFFER, B BENESOV		58	600619
DH	TA BR5		
SHCHUKAREV, S SMIR		60	200799
DH	TA BR5		
GROSS, P HAYMAN, C		62	300706
PHAS	TA2B SYST		
LEITNAKER, J BOWMA		61	700595
PHAS	TA B SYST		
NOWOTNY, H BENESOV		59	201339
PHAS	TA B SYST		
LEITNAKER, J BOWMA		61	700595
REAC	TA B SYST		
SAMSONOV, G STRASH		62	300990
VAP	TA B SYST		
HASAPIS, A MELVEGE		61	701039
MISC	TA B C SYST		
FORNEY, G J MARSHA		61	300238
COPT	TA C		
COFFMAN, J KIBLER		60	700985
COPT	TA C		
HODDAD, R E GOLDWA		49	300160
COPT	TA C		
ECKSTEIN, B FORMAN		62	300805
CRYS	TA C		
VAN ARKEL, A		24	701086
CRYS	TA C		
BOWMAN, A		61	300806
TRT	TA C		
SHAFFER, P		63	202132
MPP	TA C		
GIORGI, A SZKLARZ		63	202039
CEMP	TA C		
BITTNER, H GORETZK		62	202004
MPP	TA C		
DERGUNOVA, V KOLON		63	202026
CRYS	TA C		
BOWMAN, A		61	600836
ERES	TA C		
COOPER, J HANSLER		63	301207
VAP	TA C		
FESENKO, V BOLGAR		63	301216
DH	TA C		
HUBER, E HEAD, E		63	301248
CEMP	TA C		
INGOLD, J		63	301251
REAC	TA C		
SAMSONOV, G			301571
REAC	TA C		
SAEKI, Y OMORI, G		63	301339
THER	TA C		
SCHICK, H ANTHROP		63	301580
DH	TA C		
KORNILOV, A LEONID		62	300923
DHD	TA C		
BITTNER, H GORETZK		62	301132
MPP	TA C		
NORTON, J MOWRY, A		49	300157
PHAS	TA C		
BENESOVSKY, E RUDY		61	100181
PHAS	TA C		
NADLER, M KEMPTER		60	300301
PHAS	TA C		
SHAFFER, P		61	700941
PHAS	TA C		
SHAFFER, P		61	701067
PHAS	TA C		
NORTON, J		60	701001
PHAS	TA C		
ZALABAK, C		61	701026
PHAS	TA C		
MARTIN, R SEAGLE		61	300308
PHAS	TA C		
RYBALCHENKO, R TRE		61	300346
SPK	TA C		
COFFMAN, J KIBLER		60	700993
THER	TA C		
COFFMAN, J KIBLER		60	700993
TRT	TA C		
ZALABAK, C		61	200988
TWT	TA C		
MARTIN, R SEAGLE		61	300308
VAP	TA C		
COFFMAN, J KIBLER		60	700985
VAP	TA C		
COFFMAN, J KIBLER		60	700993
THER	TA2C		
SCHICK, H ANTHROP		63	301580
PHAS	TA2C		
KLEIN, R LEDER, L		63	301501
DF	TA CL5		
JERE, G PATEL, C		60	200850
DH	TA CL5		
SHCHUKAREV, S SMIR		60	200799
THER	TA C SYST		
CUNNINGHAM, G WARD		63	301208
PHAS	TA C SYST		
VAUGHAN, D STEWAR		60	700990
PHAS	TA C SYST		
NADLER, M KEMPTER		60	700903
REAC	TA C SYST		
SAMSONOV, G STRASH		62	300990
REAC	TA C SYST		
PORTNOI, K LEVINSK		61	300215
CPL	TA2H		
SABA, W WALLACE, W		61	300810
THER	TA HF C		
RUDY, E		63	301165
MPP	TA N		
SAMSONOV, G VERKHO		61	301573
REAC	TA N SYST		
OSTHAGEN, K KOFSTA		63	301548

CPH	TA N	NEEL, D PEARS, C	61	300146
MPP	TA N	SAMSONOV, G VERKHO	62	300997
CRYS	TA N	VAN ARKEL, A	24	701056
THER	TA2N	BOLGAR, A	61	700938
VAP	TA2N	BOLGAR, A	61	700938
PHAS	TA NI	SEEBOLD, R BIRKS	61	300295
PHAS	TA NI2	SEEBOLD, R BIRKS	61	300295
PHAS	TA3NI2	SEEBOLD, R BIRKS	61	300295
CEMP	TA NITRIDES	SAMSONOV, G	60	700947
DH	TA NITRIDES	SAMSONOV, G	60	700947
REV	TA NITRIDES	SAMSONOV, G	60	700947
ZKP	TA N SYST	GEBHARDT, E SEGHEZ	61	700646
REAC	TA N SYST	OESTHAGER, K KOFST	63	300957
PHAS	TA N SYST	VAUGHAN, D STEWAR	60	700990
MSP	TA NB SYST	AMOSOV, V M LANIS	61	300175
VAP	TA NB SYST	AMOSOV, V M LANIS	61	300175
VAP	TA O	BABELIOWSKY, T BOE	63	301179
SPK	TA O	PREMASWARUP, D	55	301323
DF	TA .	ACKERMANN, R THORN	58	601510
DHD	TA O	GOLDSTEIN, H WALSH	58	201098
DHD	TA O	WALSH, P WHITE D	58	700806
KIN	TA O	ONG, T	62	201916
SPK	TA O	PREMASWARUP, D BAR	57	600918
SPK	TA O	GRAVEN, W	61	201519
THER	TA O	SCHICK, H ANTHROP	63	301580
THER	TA O	ACKERMANN, R THORN	58	601087
THER	TA O	PEMSLER, J P	61	700650
VAP	TA O	ACKERMANN, R THORN	58	601510
DF	TA O 2	ACKERMANN, R THORN	58	601510
THER	TA O 2	SCHICK, H ANTHROP	63	301580
THER	TA O 2	ACKERMANN, R THORN	58	601087
VAP	TA O 2	ACKERMANN, R THORN	58	601510
MPP	TA O 5	SIMANOV, Y LAPITSK	54	301119
MPP	TA O 5	LAPITSKIY, A SIMAN	54	301112
SPK	TA O 5	CONLON, D DOYLE, W	61	201326
CRYS	TA2O 5	CZARNY, Z	63	301209
REAC	TA2O 5	KOFSTAD, P	63	202072
DH	TA2O 5	KORNILOV, A LEONID	62	601591
THER	TA2O 5	KORNILOV, A LEONID	62	601591
THER	TA2O 5	SCHICK, H ANTHROP	63	301580
VAP	TA2O 5	KOFSTAD, P	62	300586
REAC	TA OXIDE	BRAUER, G MULLER		301105
PHAS	TA OXIDES	WASILEWSKI, R	61	201089
KIN	TA O SYST	KOFSTAD, P	63	301506
KIN	TA O SYST	KOFSTAD, P	63	301505
PHAS	TA O SYST	BRAUER, G MUELLER	63	301196
PHAS	TA O SYST	KOUBA, L TRUNOV, V	62	301278
PHAS	TA O SYST	VAUGHAN, D STEWAR	60	700990
PHAS	TA O SYST	ANON	60	701015
PHAS	TA O SYST	KUBASCHEWSKI, O	62	601577
PHAS	TA O SYST	NORMAN, N	62	300374
PHAS	TA O SYST	NORMAN, N KOFSTAD	62	300527
VAP	TA O SYST	ANON	60	701015
ZKP	TA O SYST	HOCH, M MATHUR, M	62	300587
PHAS	TA RE SYST	BROPHY, J SCHWARZK	60	200803
KIN	TA TI SYST	VOITOVICH, R	61	201310
PHAS	TA U C SYST	BENESOVSKY, F RUDY	61	301406
PHAS	TA V SYST	EREMENKO, V TRETYA	60	201492
PHAS	TA V SYST	EREMENKO, V TRETYA	62	201711
KIN	TA W SYST	VOITOVICH, R	61	201310
PHAS	TA W C SYST	RUDY, E RUDY, E	62	300967
VAP	TA W O SYST	ANON	60	300229
PHAS	TA W RE SYST	BROPHY, J KAMDAR	61	201340
PHAS	TA ZR SYST	WILLIAMS, D JACKSO	62	301016
CPL	TB	HELTEMES, E SWENSON	61	201411
CPL	TB	LOUNASMAA, O ROACH	62	701082
CRYS	TB	KOEHLER, W WOLLAN	61	301504
ERES	TB	COLVIN, R LEGVOLD	60	601389
MPP	TB	IONOV, N MITTSEV	61	601411
SPK	TB	BURBRIDGE, E BURBR	55	601003
VAP	TB	WHITE, D WALSH, P	60	301622
VAP	TB	WHITE, D WALSH, P	61	301014
VAP	TB	WHITE, D WALSH, P	61	300455
CEMP	TB B 6	SAMSONOV, G PADERN	59	300143
PHAS	TB O	EYRING, L HOLWBERG	62	601590
CRYS	TB O 2	GRUEN, D KOEHLER	51	400545
CRYS	TB2O 3	GRUEN, D KOEHLER	51	400545
CRYS	TB O SYST	BAENZIGER, N EICK	61	300184

PHAS	TB O SYST	BAENZIGER, N C EIC	61	300184
CRYS	TC	LAM, D DARBY, J	61	601586
MISC	TC	MURIN, A N NEFEDOV	61	700574
PHAS	TC	SZABO, Z LAKATOS	62	601673
MPP	TC	EAKINS, J HUMPHRIE	63	301214
PHAS	TC	ANDERSON, E BUCKLE	60	700975
REV	TC	MURIN, A N NEFEDAV	61	700574
SPK	TC	SHADMI, Y	61	700954
THER	TC	SCHICK, H ANTHROP	62	300995
THER	TC	MARGRAVE, J	61	700967
TRT	TC	SZABO, Z LAKATOS	62	601673
SPK	TC F 6	CLAASSEN, H SELIG	62	201854
THER	TC O	SCHICK, H ANTHROP	62	300995
DH	TE	WHITE, D	61	201217
SPK	TE	NORRIS, J	60	601194
REAC	TE C	TRZEBIATOWSKI, W	62	201857
BIB	TH	DAVID, L	53	600957
CRYS	TH	AMONENKO, V VASYUT	63	301170
CEMP	TH	FRANCIS, E	58	601536
CEMP	TH	MESMARD, G UYAN, R	51	400558
CEMP	TH	RIVIERE, J	62	201806
CPH	TH	MITKINA, E	59	201029
CPH	TH	WALLACE, D C	60	300132
CPH	TH	WALLACE, D C	60	700569
CPL	TH	CLUSIUS, K FRANZOS	56	601038
CPL	TH	GRIFFEL, M SKOCHDO	53	600966
CPL	TH	SMITH, P WOLCOTT	55	601137
CPL	TH	BORELIUS, G	60	601168
CRYS	TH	SMITH, J	58	601073
CRYS	TH	DAWSON, J	52	100187
CRYS	TH	CHIOTTI, P	54	601198
CRYS	TH	ANON	57	601297
CRYS	TH	THOMPSON, J	62	201648
CRYS	TH	CHIOTTI, P	54	01227
CRYS	TH	MCCALDIN, J DUWEZ	54	600956
CTEX	TH	WILSON, W AUSTIN	56	601071
DH	TH	HOLLEY, C HUBER, E	50	601178
DH	TH	HUBER, E V HOLLEY	52	400565
ERES	TH	ANON	55	601312
ERES	TH	BENDER, D	49	601404
ERES	TH	MURK, K	69	601523
ERES	TH	BOESCHOTEN, F	59	601528
ERES	TH	BERLINCOURT, T	59	601655
ERES	TH	DANFORTH, W MORGAN	60	400535
H	TH	OELSEN, W	55	600980
KIN	TH	PETERSON, D	61	201246
MPP	TH	FRANCIS, E	58	601536
MPP	TH	MURRAY, J	58	601094
MPP	TH	SMITH, J	58	601073
MPP	TH	SKINNER, G BECKETT	50	601225
PHAS	TH	ANON	62	601629
PHAS	TH	ANON	57	601305
PHAS	TH	WILSON, W AUSTIN	56	601071
PHAS	TH	VON BOLTON, W	08	800117
PHAS	TH	MARDEN, J RENTSCHL	27	900119
PHAS	TH	SCHULTZE, A	30	900117
PHAS	TH	BADAEVA, T	61	201890
REAC	TH	DEYE, R	50	601156
REAC	TH	DEUTSCH, N ERVIN	60	500123
REAC	TH	MURRAY, J	58	601094
REV	TH	KAUFMANN, A	62	601429
REV	TH	ROLLEFSON, G HAGEM	51	601106
REV	TH	MURRAY, J	58	601094
REV	TH	KATZIN, L	56	601020
REV	TH	SANDERSON, L	61	300376
REV	TH	FRANCIS, E	58	601536
REV	TH	FRANCIS, E	58	601127
REV	TH	VETEJSKA, K	60	601187
REV	TH	RYABCHIKOV, D GOL	61	700656
SPK	TH	CHARLES	58	601084
SPK	TH	KLINKENBERG, P LANG	50	400522
SPK	TH	DAVISON, A GIACCHE	62	300823
SPK	TH	STUKENBROEKER, G M	60	601383
SPK	TH	NORRIS, J	60	601194
SPK	TH	ZABULAS, R	59	601192
SPK	TH	KLINKENBERG, P	50	400531
SPK	TH	ANON	58	601549
SPK	TH	RACAH, G	50	400547

SPK	TH		
	OSARO, F PERLMAN	52	400572
SPK	TH		
	KESSLER, D	51	400576
SPK	TH		
	EISENBERG, Y	52	400577
SPK	TH		
	TREES, R	60	600852
SPK	TH		
	VERNYL, E EGOROV	59	601189
SPK	TH		
	ELYASHEVICH, M	53	601413
SPK	TH		
	PISTORIUS, C	60	200864
SPK	TH		
	SCHUURMANS, P	46	601290
TCON	TH		
	SIDELES, P DANIELS	51	601238
THER	TH		
	SCHICK, H ANTHROP	62	300995
THER	TH		
	CHIOTTI, P	56	601324
THER	TH		
	ACKERMANN, R THORN	62	601616
THER	TH		
	PETERSON, D	61	201246
THER	TH		
	MARGRAVE, J	61	700967
THER	TH		
	SMITH, J	58	601073
THER	TH		
	DARNELL, A J MCCOL	60	700567
TRT	TH		
	MCCALDIN, J DUWEZ	54	600956
TRT	TH		
	REID, A WILMHURST	63	301556
TRT	TH		
	DEYE, K	50	601156
TRT	TH		
	SCHULTZE, A	30	900117
TRT	TH		
	MCMASTERS, O LARSE	61	800834
TRT	TH		
	MARDEN, J RENTSCHL	27	900119
VAP	TH		
	DARNELL, A	61	201182
VAP	TH		
	ACKERMANN, R THORN	62	601616
VAP	TH		
	TOSIM, S	57	601505
VAP	TH		
	DARNELL, A J MCCOL	60	700567
VAP	TH		
	MURBACH, E	57	601105
VAP	TH		
	GOLDWATER, D DANFO	60	600691
VAP	TH		
	VON BOLTON, W	08	800117
MPP	TH		
	ROUGH, F A CHUBB	60	700568
CRYS	TH B 4		
	ZALKIN, A TEMPELTO	53	100198
CRYS	TH B 4		
	ZALKIN, A TEMPLETO	50	601410
CRYS	TH B 4		
	ZALKIN, A TEMPLETO	50	400520
REV	TH B 4		
	MATTERSON, K JONES	61	300324
CEMP	TH B 6		
	LAFFERTY, J	50	400541
MPP	TH B 6		
	SAMSONOV, V ZOUNA	56	601051
REAC	TH B 6		
	SAMSONOV, V ZOUNA	56	601051
PHAS	TH BORIDES		
	BREWER, L SAWYER	50	601400
PHAS	TH B C SYST		
	TOTH, L BENESOVSKY	61	201446

PHAS	TH B O SYST		
	RASE, D	60	600872
PHAS	TH BE C SYST		
	BRISI, C ABBATTIST	61	201507
PHAS	TH BE		
	BADAEVA, T KUZNETS	61	201833
PHAS	TH BE		
	BADAEVA, T KUZNETS	61	201891
PHAS	TH C		
	KEMPTER, C KRIKORI	62	300517
REAC	TH C		
	SAMSONOV, G KASALA	60	700376
REV	TH C		
	ROUGH, F CHUBB, W	60	600610
CRYS	TH C 2		
	HUNT, G B RUNDLE	51	400573
DF	TH C 2		
	ANON	60	601337
VAP	TH C 2		
	MIKHAILOVSKII, B	63	301302
DF	TH C 2		
	MASLAN, F	59	601354
DF	TH C 2		
	ANON	59	600608
DH	TH C 2		
	PRESCOTT, C HINCKE	27	900116
PHAS	TH C 2		
	ANON	60	601414
PHAS	TH C 2		
	KEMPTER, C KRIKORI	62	300517
PHAS	TH C 2		
	PRESCOTT, C HINCKE	27	900116
THER	TH C 2		
	ANON	60	601458
THER	TH C 2		
	ANON	60	601414
TRT	TH C 2		
	PRESCOTT, C HINCKE	27	900116
MPP	TH CARBIDES		
	SKINNER, G BECKETT	50	601225
REAC	TH CARBIDES		
	WILHELM, H CHIOTTI	49	400536
PHAS	TH C SYST		
	ROGERS, B	50	601266
PHAS	TH C SYST		
	MICKELSON, R PETER	57	601057
PHAS	TH C SYST		
	CHIOTTI, P	52	100204
PHAS	TH C SYST		
	WILHEM, H CHIOTTI	50	400521
TRT	TH C SYST		
	WILHEM, H CHIOTTI	50	400521
TRT	H C SYST		
	CHIOTTI, P	52	100204
BIB	TH C SYST		
	COMSTOCK, M	60	600623
PHAS	TH CE		
	BADAEVA, T KUZNETS	61	201897
PHAS	TH CE LA SYST		
	EVANS, D RAYNOR, G	62	201812
SPK	TH I		
	ZABULAS, R	59	601192
PHAS	TH F 4		
	KIRSHENBAUM, A	61	201183
PHAS	TH MMSYST		
	MCMASTERS, O PALME	62	301535
PHAS	TH MO C		
	RUDY, E BENESOVSKY	63	301566
PHAS	TH MO C SYST		
	RUDY, E BENESOVSKY	63	301332
REAC	TH MG SYST		
	UNSWORTH, W	60	200876
CRYS	TH N		
	CHIOTTI, P	52	601237
THEO	TH N		
	BAUGHAN, E	59	300866
TRT	TH N		
	CHIOTTI, P	52	601237

BIB	TH N	COMSTOCK, M	60	600623
CPH	TH3N 4	SATO, S	39	900114
DH	TH3N 4	NEUMANN, B KROGER	32	900113
MPP	TH NITRIDES	SKINNER, G BECKETT	60	601226
DF	TH O	ACKERMANN, R THORN	58	601510
PHAS	TH O	KORNILOV, I	60	200769
SPK	TH O	ROSEN, B	62	301560
THER	TH O	SCHICK, H ANTHROP	62	300995
THER	TH O	ACKERMANN, R THORN	58	601087
VAP	TH O	ACKERMANN, R THORN	58	601510
THER	TH O 2	ACKERMAN, E. RAUH	63	301164
CPH	TH O 2	HOCH, M JOHNSTON	61	201171
CPH	GH O 2	HOCH, M JOHNSTON,	61	700658
REAC	TH O 2	KOMAREK, K COUCOUL	63	301269
TRT	TH O 2	MUMPTON, F ROY, R	60	301308
CPL	TH O 2	OSBORNE, D WESTRUM	53	600968
CRYS	TH O 2	DRAPER, A MILLIGAN	59	201104
CRYS	TH O 2	VAN ARKEL, A	24	701066
CRYS	TH O 2	VOGEL, R KEMPTER	59	601177
CTEX	TH O 2	SKINNER, B	57	601065
CTEX	TH O 2	GRAIN, C CAMPBELL	61	601471
CTEX	TH O 2	KEMPTER, C ELLIOTT	59	601160
DF	TH O 2	ACKERMANN, R THORN	58	601510
DH	TH O 2	VON WARTENBERG, H	09	900108
DH	TH O 2	CHAUVENET, E	11	900109
ELCH	TH O 2	DANFORTH, W	57	601317
ERES	TH O 2	VAN ARKEL, A FLOOD	53	600950
MSP	TH O 2	HASAPIS, A MELVEGE	61	701017
MPP	TH O 2	NAGASAWA, S	50	400530
PHAS	TH O 2	GRAIN, C CAMPBELL	61	601471
PHAS	TH O 2	RUFF, O EBERT, F	29	900120
SPK	TH O 2	COFFMAN, J KIBLER	60	700993
SURF	TH O 2	DRAPER, A MILLIGAN	59	201104
TCON	TH O 2	ADAMS, M	54	600961
TCON	TH O 2	NORTON, H KINGERY	52	601240
TCON	TH O 2	WOCHMAN, J	62	601472
TCON	TH O 2	KINGERY, W FRANCL	54	600971
THER	TH O 2	COFFMAN, J KIBLER	60	700993
THER	TH O 2	ACKERMANN, R THORN	58	601087
THER	TH M2	VICTOR, A DOUGLAS	61	201108
THER	TH O 2	INGHRAM, M CHUPKA	57	601067
THER	TH O 2	KUBASCHEWSKI, O	61	600792
THER	TH O 2	ZAREMBO, Y	61	201449
TRT	TH O 2	RUFF, O EBERT, F	29	900120
VAP	TH O 2	SHAPIRO, E	52	100186
VAP	TH O 2	COFFMAN, J KIBLER	60	700993
VAP	TH O 2	ACKERMANN, R THORN	56	600983
VAP	TH O 2	DARNELL, A	61	201182
VAP	TH O 2	ACKERMANN, R THORN	58	601510
VAP	TH O 2	ACKERMANN, R	56	601267
VAP	TH O 2	HASAPIS, A PANISH	60	600667
VAP	TH O 2	HOCH, M JOHNSTON	54	600972
CRYS	TH OXIDES	FRIED, S	56	601021
BIB	TH O SYST	COMSTOCK, M	60	600623
PHAS	TH O SYST	WESTRUM, E GRONVOL	62	601613
THER	TH O SYST	WESTRUM, E GRONVOL	62	601613
THER	TH O SYST	ACKERMANN, R THORN	62	601616
VAP	TH O SYST	WESTRUM, E GRONVOL	62	601613
VAP	TH O SYST	ACKERMANN, R THORN	62	601616
REAC	TH O AL SYST	RALEIGH, D	62	201698
PHAS	TH RH	FERRO, R RAMBALDI	61	201696
REAC	TH U	ENGLE, G GOEDDEL	62	201525
PHAS	TH U B SYST	TOTH, L NOWOTHNY	61	201405
PHAS	TH U C SYST	IVANOV, O ALEKSEEV	61	201875
THEO	TH U C SYST	BENESOVSKY, F RUDY	61	900203
PHAS	TH V	PALMER, P MCMASTER	62	201791
PHAS	TH W C	RUDY, E BENESOVSKY	62	201628
CRYS	TH Y SYST	EVANS, D RAYNOR, G	60	200874
PHAS	TH ZN SYST	CHIOTTI, P GILL, K	61	700624
THER	TH ZN SYST	CHIOTTI, P GILL, K	61	700624
PHAS	TH ZR	BADAEVA, T ALEKSE	61	201892
PHAS	TH ZR C SYST	BODAEVA, T KUZNETS	63	202006
PHAS	TH ZR C SYST	RUDY, E BENESOVSKY	62	300969
PHAS	TH ZR V SYST	BADAEVA, T ALEKSEE	61	201893
CPH	THEORY	FOMICHEV, E KANDYB	62	300885
DF	THEORY	MAZO, R	63	202100
CPH	THEORY	DIDENKO, V YARYSHE	63	301135
CPH	THEORY	DIDENKO, V YARYSHE	62	300878

CPH	THEORY		
CHAMBERS, R		62	300819
CPL	THEORY		
FOREMAN, A		62	301083
CPL	THEORY		
RELLER, J WALLACE		62	301092
CPL	THEORY		
MARADNDIN, A FLINN		61	301085
CPL	THEORY		
MARADNDIN, A FLINN		61	301084
CRYS	THEORY		
RAU, R		61	201198
DH	THEORY		
WILCOX, D		62	301011
DH	THEORY		
REZNITSKII, L		61	300348
DHD	THEORY		
VERHAEGEN, G STAFFO		62	301050
H	THEORY		
FOMICHEV, E KANDYB		62	300885
MISC	THEORY		
SAMSONOV, G KOVALC		62	301164
MSP	THEORY		
GOROKHOV, L		62	300895
PHAS	THEORY		
JONES, G		63	301490
PHAS	THEORY		
BOROVSKII, I MARCH		60	201014
VAP	THEORY		
ICZKOWSKI, R MARGR		63	300905
VAP	THEORY		
GREGORY, N		63	300892
VAP	THEORY		
MARTYNKEVICH, G		61	300554
ZKP	THEORY		
WREDERKEHR, R		62	301056
BIB	THERMODYNAMICS		
LATIMER, W		54	601635
PHAS	THERMODYNAMICS		
RUDY, E		62	900228
REAC	THERMODYNAMICS		
WAHLBECK, P EDWARD		61	301163
REV	THERMODYNAMICS		
BAZAROV, I		62	301185
REV	THERMODYNAMICS		
WELLS, P		63	301618
REV	THERMODYNAMICS		
SKINNER, H WADDING		63	301589
THEO	THERMODYNAMICS		
RUDY, E		63	301565
THEO	THERMODYNAMICS		
ANTHONY, R HIMMELB		63	301398
THEO	THERMODYNAMICS		
MASLOV, P MASLOV		61	300658
THEO	THERMODYNAMICS		
STORONKIN A SHULT		60	300296
THEO	THERMODYNAMICS		
BAZAROV, I		61	300389
THEO	THERMODYNAMICS		
MAYER, J		62	300397
THEO	THERMODYNAMICS		
PRILEZHAEVA, N		60	301153
THER	THERMODYNAMICS		
MEIXNER, J		60	200824
VAP	THERMODYNAMICS		
BLANC, B		61	201346
BETA	TI		
KRUPNIKOU, K BAKAN		63	301149
BIB	TI		
WOHLL, M		60	700723
CPH	TI		
FIELDHOUSE, I LANG		60	601583
CPH	TI		
SEREBRENNIKOV, N N		61	300192
CPL	TI		
CLUSIUS, K FRANZOS		58	200927
CPL	TI		
STALINSKI, B BIEGA		61	201045
CPL	TI		
STARKE, E CHENG, C		62	201730
CRYS	TI		
ANDERSON, S		60	200845
CRYS	TI		
SADOVSKII, V BOGAC		60	600863
CRYS	TI		
SOREL, M			600787
CRYS	TI		
JAMIESON, J		63	301263
CPL	TI		
KNIEF, G BETTERTON		63	301264
CRYS	TI		
WOOD, R		62	201956
CTEX	TI		
FIELDHOUSE, I LANG		60	601583
CTEX	TI		
BESSERER, C		58	700929
CTEX	TI		
NOWOTNY, H LAUBE		61	600844
CTEX	TI		
WILLIAMS, D		61	600782
CTEX	TI		
WASILEWSKI, R		61	201342
DH	TI		
GOLDSMITH, A HIRSC		60	700930
DHT	TI		
HERTZRICKEN, S SLY		62	300708
ERES	TI		
BRIDGMAN, P		51	400533
ERES	TI		
BERLINCOURT, T		59	601655
ERES	TI		
POWELL, R W TYE, R		61	700652
ERES	TI		
WASILEWSKI, R		62	201515
KIN	TI		
KOXSTAD, P ANDERSO		61	700531
KIN	TI		
ARZHANYI, P VOLKOV		62	201975
MISC	TI		
SPINK, D		61	200891
CPH	TI		
HOLLAND, M		63	202054
MPP	TI		
KAREV, V KLYUCHARE		63	202064
ERES	TI		
KORNILOV, I MIKHEE		63	202079
CRYS	TI		
NIKIFOROV, I SACHE		63	202109
CPL	TI		
SHIMIZU M TAKAHAS		63	202135
REV	TI		
SHVARTS, G SAVEIKI		63	202136
MISC	GI		
WADSLEY, A		61	201100
MISC	TI		
BASKIN, M TRETYAKO		62	201951
MPP	TI		
BESSERER, C		58	700929
MPP	TI		
SKINNER, G BECKETT		50	601225
PHAS	TI		
KORNILOV, I		60	200907
PHAS	TI		
GOLDSMITH, A HIRSC		60	700930
PHAS	TI		
WORNER, H		60	200991
PHAS	TI		
SOREL, M			600787
PHAS	TI		
NISHIMURA, H HIRAM		57	201397
PHAS	TI		
BLOK, N GLAZOVA, N		61	201490
PHAS	TI		
KUSAMICHI, H KUSAM		57	201494
PHAS	TI		
WYDER, W HOCH, M		62	201581

		SAVITSKII, E LIVAN	61	201889
PHAS	TI	SEMENCHENKOV, A	61	201894
REAC	TI	BIRYUKOVA, L SAKSO	60	200851
REAC	TI	LAINER, D TSYPIN	61	201134
REAC	TI	KOFSTAD, P ANDERSO	61	201098
REAC	TI	OGURTSOV, S	60	200967
REAC	TI	STRINGER, J	60	700559
REAC	TI	ANITOVA, I S GARBA	61	700603
REAC	TI	CERVONE, E FURLANI	61	201521
REAC	TI	ANDREEVA, V ALEKSE	62	201814
REV	TI	WOHLL, M	60	701053
REV	TI	EREMENKO, U	60	300286
REV	TI	BOMBERGER, H	62	300369
SPK	TI	ZHURAKOVSKII, E VA	59	201226
SPK	TI	ROSENZWEIG, N PORT	60	700996
SPK	TI	ROSENZWEIG, N PORT	60	700901
SPK	TI	SWEENEY, W SEAL, R	61	201112
SPK	TI	WILSON, C THEKAEKA	61	201001
SPK	TI	SHAW, C	56	600908
SPK	TI	BLOKHIN, M SHUVAEV	62	201778
SPK	TI	BOLOTIN, G VOLOSHI	62	201830
TCON	TI	FIELDHOUSE, I LANG	60	601583
TCON	TI	LOWRIE, R	61	700943
TCON	TI	BESSERER, C	58	700929
TCON	TI	POWELL, R W TYE, R	61	700652
TCON	TI	KUPROVSKII, B GELD	61	201867
THEO	TI	ROSENZWEIG, N PORT	60	700996
TRT	TI	BOKSHTEIN, S GUBAR	62	301408
TRT	TI	JAYARAMAN, A KLEME	63	301482
VAP	TI	SCHRAM, A	60	301583
VAP	TI	FRANZEN, J HINTENB	61	700970
VAP	TI	HANLIN, H	60	700951
VAP	TI	GOLDSMITH, A HIRSC	60	700930
KIN	TI SYST	KUBASCHEWSKI, O	62	601577
THER	TI SYST	KUBASCHEWSKI, O	62	601577
CPH	TI B 2	KRESTOVNIKOV, A VE	60	300672
VAP	TI B 2	FESENKO, V BOLGAR	63	301216
CRYS	TI B 2	GORELIK, C ELYUTIN	62	301230
THER	TI B 2	MIKSIC, M	63	301303
KIN	TI B 2	RAKOVSKII, V	62	301326
REAC	TI B 2	FUNKE, V YUDKOVSKI	63	202034
MPP	TI B 2	MALYUCHKOV, O POVI	62	202096
CRYS	TI B 2	EHRLICH, P GUTSCHE	61	201331
CTEX	TI B 2	GILMAN, J ROBERTS	61	300300
DF	TI B 2	KRESTOVNIKOV, A VE	60	300672
DH	TI B 2	LOWRIE, R	61	700956
DH	TI B 2	LOWELL, C WILLIAMS	61	300410
DH	TI B 2	EPELBAUM, V A STAR	56	300194
DH	TI B 2	WILLIAMS, W	61	300523
DHT	TI B 2	LOWRIE, R	61	700956
H	TI B 2	MEZAKI, R TILLEUX	62	601617
MPP	TI B 2	PORTNOY, K SAMSONO	61	300486
MPP	TI B 2	SHCHERBAKOV, V VEY	60	300984
MPP	TI B 2	BLUM, A WIELCZKO	61	300491
MSP	TI B 2	LOWRIE, R	61	700956
MSP	TI B 2	LOWRIE, R	60	701014
PHAS	TI B 2	FORELIK, C YELYUTI	62	300884
PHAS	TI B 2	LEITNAKER, J KRIKO	62	300408
REAC	TI B 2	LEITNAKER, J KRIKO	62	300408
REAC	TI B 2	LAVENDEL, H	61	300482
REAC	TI B 2	KUBO, T HANAZAWA	60	201428
S	TI B 2	MEZAKI, R TILLEUX	62	601617
THER	TI B 2	BOLGAR, A	61	700938
THER	TI B 2	MEERSON, G	60	300298
VAP	TI B 2	BOLGAR, A	61	700938
VAP	TI B 2	LOWRIE, R	61	700956
VAP	TI B 2	LOWRIE, R	60	701014
VAP	TI B 2	SCHICK, H ANTHROP	63	300994
VAP	TI B 2	KIBLER, G LYON, T	61	300409
REAC	TI BORIDES	SAMSONOV, G	59	600120
MSP	TI B SYST	SEARCY, A WILLIAMS	60	300590
VAP	TI B SYST	SCHISSEL, P TRULSO	62	300606
PHAS	TI B C SYST	NOWOTNY, H	61	201170
REAC	TI B C SYST	SAMSONOV, G	60	300273
MISC	TI B N	FORNEY, G J MARSHA	61	300238
PHAS	TI B N SYST	NOWOTNY, H	61	201170
SPK	TI BE	VAINSHTEIN, E BLOK	62	201585
PHAS	TI BE SYST	VAINSHTEIN, E	61	201163

THER	TI BR	FUNAKI, K UCHIMURA	61	201609
CEMP	TI C	BONDARENKO, B ERMA	62	301409
DF	TI C	VIDALE, G	61	301610
DHD	TI C	BITTNER, H GORETZK	62	301132
CRYS	TI C	GORELIK, C ELYUTIN	62	301230
TCON	TI C	HOCH, M VARDI, J	63	301245
CEMP	TI C	INGOLD, J	63	301251
DH	TI C	KHRIPUN, M ARIYA	62	301258
CTEX	TI C	KRIKORIAN, WALLA	63	301285
CRYS	TI O	HOCH, M	63	202053
CRYS	TI C	ASHBEE, K EELES, W	62	201994
CEMP	TI C	BITTNER, H GORETZK	62	202004
MPP	TI C	AGTE, C BLUM, G	61	300342
REAC	TI C	SAMSONOV, G		301571
TCON	TI C	HOCH, M VARDI, J	63	301476
VAP	TI C	VIDALE, G	61	301611
VAP	TI C	ANON	60	600666
PHAS	TI C	ARAI ZENZABURO HA	60	200773
THER	TI .	BOLGAR, A	61	700938
VAP	TI C	BOLGAR, A	61	700938
COPT	TI C	BRESKER, R VORONIN	59	300799
COPT	TI C	COFFMAN, J COULSON	61	701040
CRYS	TI C	COFFMAN, J COULSON	61	701040
DF	TI C	COFFMAN, J COULSON	61	701040
PHAS	TI C	COFFMAN, J COULSON	61	701040
VAP	TI C	COFFMAN, J COULSON	61	701040
DF	TI C	COFFMAN, J COULSON	61	300293
REAC	TI C	EREMENKO, V VELIKA	59	201279
PHAS	TI C	FORELIK, C YELYUTI	62	300884
DH	TI C	FUJISHIRO, S GOKCE	61	701012
THER	TI C	FUJISHIRO, S GOKCE	61	701012
VAP	TI C	FUJISHIRO, S GOKCE	61	701012
CTEX	TI C	GILMAN, J ROBERTS	61	300300
PHAS	TI C	GORBUNOV, N ET AL	61	300382
REAC	TI C	GRIGOREVA, V SERED	61	300398
COPT	TI C	HODDAD, R E GOLDWA	49	300160
REAC	TI C	HOLDEN, F A KINGER	55	300161
CEMP	TI C	HOLLANDER, L E JR	61	700528
ERES	TI C	HOLLANDER, L E JR	61	700528
S	TI C	KAUFMAN, L	62	300910
KIN	TI C	KIRILLOVA, G MEERS	60	200759
KIN	TI C	KUBO, K SHINRIKI	60	201210
DH	TI C	LOWELL, C WILLIAMS	61	300410
PHAS	TI C	MARTIN, R SEAGLE	61	300308
TRT	TI C	MARTIN, R SEAGLE	61	300308
DH	TI C	MOROZOVA, M KHRIPU	62	300597
CPH	TI C	NEEL, D PEARS, C	61	300146
REAC	TI C	NIKOLAISKI, E	60	300130
CEMP	TI C	NOGUCHI, S SATE, T	60	300227
MPP	TI C	NORTON, J MOWRY, A	49	300157
PHAS	TI C	NORTON, J	60	701001
REAC	TI C	OGAWA, K BRANDO, Y	59	201332
CRYS	TI C	RAMAN, S RAMACHAND	62	300561
MPP	TI C	SUGIYAMA, M SUZUKI	61	300331
TCON	TI C	TAYLOR R	61	201288
CRYS	TI C	VAN ARKEL, A	24	701056
THER	TI C 2	MEERSON, G	60	300298
REAC	TI CARBIDES	MEERSON, G ZELIKMA	61	201912
MPP	TI C SYST	BASKIN, M TRETYAKO	61	300856
PHAS	TI C SYST	BICKERDIKE, R L HU	59	300156
MPP	TI C SYST	BURYLEV, B	61	301071
THER	TI C SYST	CUNNINGHAM, G WARD	63	301208
PHAS	TI C SYST	EDWARDS, R RAINE	52	300288
PHAS	TI C SYST	KURMAKOV, N TRONEV	61	601588
PHAS	TI C SYST	MAYRU[illegible]H, D OGDEN	60	700983
REAC	TI C SYST	PORTNOI, K LEVINSK	61	300215
PHAS	TI C CO SYST	EREMENKO, V LESNIK	56	300285
PHAS	TI C MO SYST	EREMENKO, V VELIKA	61	201278
PHAS	TI C NB SYST	YELYNTIN, V BERNST	55	300283
MPP	TI C NI SYST	KORNILOV, N PRYAKH	60	300209
PHAS	TI C NI SYST	EREMENKO, V N KOSO	59	300212
CEMP	TI C N SYST	LVOV, S NEMCHENKO	62	201673
PHAS	TI C W SYST	KREIMER, G VAKHOVS	59	300213
REAC	TI CL	GOPIENKO, V	60	200913
THER	TI CL3	CLIFTON, D MACWOOD	56	300292
TRT	TI CL3	OGAWA, S	60	200764
VAP	TI CL3	SANDERSON, B MACWO	56	300291
REAC	TI CL4	KRIEVE, W MASON, D	56	300290

S	TI CL4		
MUNSTER, A RICH, G		56	300320
THER	TI CL4		
KRESTOVNIKOV, A VE		59	200783
THER	TI CL4		
NIEDERKORN, I		60	201771
ZKP	TI CL4		
MUNSTER, A RICH, G		56	300320
MPP	TI CR B SYST		
MEYERSON, G		59	301115
PHAS	TI CR SYST		
GOLUBTSOVA, R		61	201150
PHAS	TI CR SYST		
ERMANIS, F FARRER		61	201240
CPL	TI F 4		
EULER, R WESTRUM		61	201157
DH	TI F 4		
GREENBERG, E SETTL		62	300739
VAP	TI FE O SYST		
WEBSTER, A H BRIGH		61	300164
THER	TI HALIDES		
KING, E WELLER, W		61	300735
PHAS	TI H SYST		
LIVANOV, V BUKHANO		61	300386
REAC	TI I		
FUNAKI, K UCHIMURE		61	201688
PHAS	TI IR		
CROENI, J ARMANTRO		62	201972
PHAS	TI MN		
WATERSTRAT, R DAS		62	201702
CPL	TI MO SYST		
HAKE, R		61	201456
CRYS	TI MO SYST		
DUPOUY, J AVERBACH		61	201180
PHAS	TI MO SYST		
KORNILOV, I POLYAK		61	201242
VAP	TI MO SYST		
KUZMIN, A PALATNIK		62	300922
MPP	TI N		
SAMSONOV, G VERKHO		61	301573
REAC	TI N		
SCHAEFER, H FUHR		62	301578
REAC	TI N		
ORBACH, H		62	301547
THEO	TI N		
GOWARD, G HERSHENS		63	202042
VAP	TI N		
FESENKO, V BOLGAR		63	301216
VAP	TI N		
AKISHIN, P KHODEEV		62	300592
PHAS	TI N		
ARAI ZENZABURO HA		60	200773
THEO	TI N		
BAUGHAN, E		59	300866
THER	TI N		
BOLGAR, A		61	700938
VAP	TI N		
BOLGAR, A		61	700938
KIN	TI N		
DOUGLASS, D ST PIE		61	201341
VAP	TI N		
DREGER, L MARGRAVE		60	700991
VAP	TI N		
DREGER, L		62	300720
VAP	TI N		
DREGER, L		61	300528
VAP	TI N		
DREGER, L MARGRAVE		60	600641
S	TI N		
KAUFMAN, L		62	300910
CRYS	TI N		
LOWRIE, R		60	701014
S	TI N		
MUNSTER, A RICH, G		56	300320
ZKP	TI N		
MUNSTER, A RICH, G		56	300320
PHAS	TI N		
NEVITT, M DOWNEY,		60	200875
CRYS	TI N		
PEARSON, W		62	301029
SPK	TI N		
PHILIPP, W		62	300521
CEMP	TI N		
SAMSONOV, G VERKHO		62	300731
MPP	TI N		
SAMSONOV, G VERKHO		61	300203
MPP	TI N		
SAMSONOV, G VERKHO		61	201264
MPP	TI N		
SAMSONOV, G VERKHO		62	300997
REAC	TI N		
FEDOSEEV, V NEMKOV		62	201757
CEMP	TI N		
SAMSONOV, G FOMENK		63	202128
TRT	TI N		
SAMSONOV, G FOMENK		63	202128
SPK	TI N		
PARKINSON, W		63	202115
CRYS	TI N		
VAN ARKEL, A		24	701056
CEMP	TI NITRIDES		
SAMSONOV, G		60	700947
DH	TI NITRIDES		
SAMSONOV, G		60	700947
REV	TI NITRIDES		
SAMSONOV, G		60	700947
CRYS	TI N SYST		
HOLMBERG, B		62	300594
PHAS	TI N SYST		
MAYRUTH, D OGDEN,		60	700983
MPP	TI N SYST		
HARVEY, J KAUFMANN		59	600640
ERES	TI N SYST		
WASILEWSKI, R		62	301075
PHAS	TI NB SYST		
SHAKHOVA, K BUDBER		61	201234
PHAS	TI NB CR SYST		
SHAKHOVA, K BUDBER		62	300993
PHAS	TI NB V SYST		
KORNILOV, I VLASOV		57	500126
PHAS	TI NB ZR SYST		
MIKHEEV, V BELOUSO		61	300834
CRYS	TI NI SYST		
BARTON, J PURDY, G		60	300210
PHAS	TI NI SYST		
POOLE, D M HUME, W		55	300208
PHAS	TI NI SYST		
BARTON, J PURDY, G		60	300210
PHAS	TI NI SYST		
PURDY, G PARR, J		61	300279
CRYS	TI O		
HOCH, M		63	301477
CRYS	TI O		
POPOV, YU		62	301321
CRYS	TI O		
ANDERSON, S		60	200845
SPK	TI O		
BERG, R A SINANOGL		60	300177
ERES	TI O		
SAMOKHVALOV, A RUS		63	301567
ERES	TI O		
MCLAREN, G		62	301534
ERES	TI O		
YAMASHITA, J		63	301625
SPK	TI O		
ROSEN, B		62	301560
THER	TI O		
HOCH, M		61	301475
MISC	TI O		
BLAIR, L R BEACHAM		53	300150
SPK	TI O		
PRASAD, S		63	202120
SPK	TI O		
WALLACE, I BEARDSL		61	202157
TRT	TI O		
WANG, C GRANT, N		56	202158

PHAS	TI O	BREWER, L MASTIK	49	601634
PHAS	TI O	TROJER, F	62	201929
PHAS	TI O	PETTERSON, A LINDG	62	301162
CRYS	TI O	CODLING, K	61	600776
SPK	TI O	FRASER, P A JERMAI	54	300145
DF	TI O	HOCH, M	60	300311
S	TI O	HOCH, M IYER, A	62	300897
S	TI O	KAUFMAN, L	62	300910
SPK	TI O	KIESS, C	48	600685
PHAS	TI O	KORNILOV, I	60	200769
DH	TI O	KRESTOVNIKOV, A	62	300930
TCON	TI O	KURYLENKO, C	58	201566
MPP	TI O	LECERF, A	62	300939
REAC	TI O	MAKAROV, E KUZNETS	60	600772
SPK	TI O	ORTENBURG, F	60	600917
SPK	TI O	ORTENBERG, F	61	300821
SPK	TI O	PAPOUSEK D	61	700676
THER	TI O	PAPOUSEK I	61	700675
SPK	TI O	PARKINSON W NICHO	59	600612
SPK	TI O	PETTERSSON A LIND	61	700544
SPK	TI O	PETTERSSON A N LI	61	700605
SPK	TI O	PHILLIPS, J G	54	300165
SPK	TI O	PHILLIPS J	50	600890
SPK	TI O	PHILLIPS, J	51	600891
ERES	TI O	WASILEWSKI, R	62	201516
CRYS	TI O	STRAUMANIS, M LI	60	200780
CEMP	TI O 2	GREENER, E WHITMOR	61	600862
CRYS	TI O 2	KOFSTAD P	62	301607
CRYS	TI O 2	ASHBEE, K EELES, W	62	201994
PHAS	TI O 2	DACHILLE, F ROY, R	62	202022
PHAS	TI O 2	DIAMOND, J SCHNEID	60	202028
CEMP	TI O 2	ACKET, G VOLGAR, J	63	301165
CPH	TI O 2	JOSHI, S MITRA, S	60	200767
CPL	TI O 2	JOSHI, S MITRA, S	60	200767
CRYS	TI O 2	YOGANARASIMHAN, S	61	200881
CRYS	TI O 2	ANDERSON, S	60	200845
CRYS	TI O 2	STRAUMANIS, M EJIM	61	201078
CRYS	TI O 2	VON WERNER, H BAUR	56	300181
CRYS	TI O 2	RAO, C YOGANARASMH	61	700535
CRYS	TI O 2	RAO, C	61	700549
CRYS	TI O 2	BAUR, W H	61	700555
CTEX	TI O 2	GRAIN, C CAMPBELL	61	601471
ELCH	TI O 2	SMIRNOV, M PALGNEV	60	300297
ERES	TI O 2	GREENER, E WHITMOR	61	300487
KIN	TI O 2	MOROZOV, I STEFANY	58	200796
KIN	TI O 2	KENNEDY, D R RITCH	58	300225
KIN	TI O 2	SUZUKI, A KOTENA	62	201838
PHAS	TI O 2	BRAUER, J LITTKE	60	201990
PHAS	TI O 2	DELIMARSKY, Y BUDE	62	300880
PHAS	TI O 2	KNOLL, H	63	301266
REAC	TI O 2	KOMAREK, K COUCOUL	63	301269
CPL	TI O 2	MATOSSI, F	63	301299
MPP	TI O 2	BAUR, W H	61	700554
PHAS	TI O 2	GRAIN, C CAMPBELL	61	601471
PHAS	TI O 2	STRAUMANIS, M EJIM	61	201078
PHAS	TI O 2	IIDA Y OZAKI, S	61	700519
PHAS	TI O 2	RAO, C YOGANARASMH	61	700535
PHAS	TI O 2	COCCO, A VIRDIS, P	61	201316
PHAS	TI O 2	MASSAZZA, F	61	201293
REAC	TI O 2	MELENTEV, B	60	200964
REAC	TI O 2	KUTSEV, V S ORMONT	56	300153
REAC	TI O 2	GEBHARDT, J HERRIN	58	300217
REAC	TI O 2	MEERSON, G	62	300950
REV	TI O 2	PETER, A	62	201523
REAC	TI O 2	CZANDE[illegible]NS, A W HOM	59	300224
MPP	TI O 2	MCTAGGART F	63	202101
MPP	TI O 2	NAGARJAN, G	63	202106
REV	TI O 2	GRANT, F	59	300890
SPK	TI O 2	PRASAD, S	62	301553
SPK	TI O 2	SOFFER, B	61	201327
THER	TI O 2	KUBASCHEWSKI, O	61	600792
THER	TI O 2	SCHICK, H ANTHROP	63	301579
THER	TI O 2	SCHICK, H ANTHROP	63	301580
TRT	TI O 2	RUDNEVA, A MODEL	63	301564
TRT	TI O 2	BRAUER, J LITTKE	60	201990
TRT	TI O 2	RAO, C YOGANARASMH	61	700535
TRT	TI O 2	RAO, C	61	700549
ZKP	TI O 2	KUTSEV, V S ORMONT	55	300153

PHAS	TI2O 3	BRAUER, J LITTKE,R	60	200777
TRT	TI2O 3	BRAUER, J LITTKE,R	60	200777
MPP	TI2O 3	LECERF, A	62	300939
CRYS	TI2O 3	STRAUMANIS, M EJIM	62	300692
ERES	TI2O 3	YAHIA, J FREDERIKS	61	300490
CRYS	TI2O 3	ABRAHAMS, S	63	201991
E	TI2O 3	ARIYA, S SOBOLEVA	61	300787
PHAS	TI3O	KORNILOV, I GLAZOV	63	202081
CRYS	TI3O 5	ASBRINK, S MAGNELI	59	700522
CRYS	TI5O 9	ANDERSSON, S	60	201381
PHAS	TI6O	KORNILOV, I GLAZOV	63	202081
BIS	TI OXIDES	CHAPMAN, M	60	701005
CRYS	TI OXIDES	MAGNELI, A ANDERSO	61	201566
KIN	TI OXIDES	DOUGLASS, D ST PIE	61	201341
PHAS	TI OXIDES	ANDERSSON, S	59	201178
VAP	TI O SYST	FRANZEN, H	63	202033
THEO	TI O SYST	GELD, P TSKHAI, V	63	202036
THER	TI O SYST	VEINBACHS, A KOMAR	62	601611
ERES	TI O SYST	WASILEWSKI, R	62	301075
PHAS	TI O SYST	MAYRUTH, D OGDEN	60	700983
CEMP	TI O SYST	VASILEV, Y KHRYCH	63	301608
CPH	TI O SYST	NOMURA, S KAWAKUBO	61	700638
PHAS	TI O SYST	LIVANOV, V BUKHANO	61	300386
CRYS	TI O SYST	MAGNELI, A	60	600617
PHAS	TI O SYST	KUBASCHEWSKI, O	62	601577
THER	TI O SYST	KRESTOVNIKOV, A LO	60	300927
CRYS	TI O SYST	HOLMBERG, B	62	300596
REAC	TI O SYST	HURLEN, T	60	200890
CPH	TI O SYST	EROFEEVA, M LUKINY	61	700602
CRYS	TI O SYST	BRIGHT, N	61	300661
CRYS	TI O SYST	BRIGHT, N	61	300661
PHAS	TI O SYST	BLUMENTHAL, R WHIT	62	601666
THER	TI O SYST	BLUMENTHAL, R WHIT	62	601666
CRYS	TI O SYST	ARIYA, S POPOV, Y	62	300599
VAP	TI O SYST	ANON	60	701015
PHAS	TI O SYST	ANON	60	701015
CRYS	TI O 2 SYST	VOTINOV, M DEMIDEN	62	301613
REAC	TI O C	KUBO, T SHINRIKI	61	201691
PHAS	TI O C SYST	NISHIMURA, H KIMUR	54	300169
REAC	TI O C SYST	NISHIMURA, H KIMUR	54	300169
PHAS	TI RE	AGEEV, N KARPINSKI	61	201762
PHAS	TI SC SYST	SAVITSKII, E BURKH	61	700622
DH	TI SI SYST	GOLUTVIN, Y	56	400599
DH	TI SI SYST	GOLUTVIN, Y	62	301229
PHAS	TI SI SYST	GOLUBTSOVA, R B	61	300174
PHAS	TI SI O SYST	COCCO, A SCHROMEK	60	201188
CPL	TI V SYST	CHENG, C GUPTA, K	62	300760
PHAS	TI V SYST	ERMANIS, F FARRER	61	201240
PHAS	TI V SYST	KORNILOV, I POLYAK	61	201242
MPP	TI W B SYST	MEYERSON, G	59	301115
CRYS	TI W C SYST	FUNKE, V PANOV, V	61	201236
MPP	TI W C SYST	FUNKE, V PANOV, V	61	201236
PHAS	TI W C SYST	FUNKE, V PANOV, V	61	201236
PHAS	TI Y SYST	BARE, D	61	201145
PHAS	TI ZR SYST	ENCE, E MARGOLIN	61	200919
PHAS	TI ZR SYST	ENCE, E MARGOLIN	61	300162
PHAS	TI ZR SYST	GRIDNEV, V TREFILO	60	201093
PHAS	TI ZR O SYST	HOCH, M	59	201136
REAC	TI ZR O SYST	RUH, R	63	202124
PHAS	TI ZR O SYST	HOCH, M DEAN, R	61	300545
THER	TI ZR O SYST	HOCH, M DEAN, R L	59	300214
THER	TI ZR O SYST	HOCH, M DEAN, R	61	300545
PHAS	TI ZR O SYST	DOMAGALA, R		300302
CRYS	TM	KOEHLER, W WOLLAN	61	301504
DH	TM	SAVAGE, W HUDSON	59	601126
ERES	TM	COLVIN, R LEGVOLD	60	601389
SPK	TM	SAKELLARIDIS, P	53	100184
SPK	TM	AKIMOV, A	57	601099
SPK	TM	MERRILL, P GREENST	56	601007
VAP	TM	ANON	56	601319
SPK	TM	BLAISE, J VETTER	63	202005
VAP	TM	SAVAGE, W HUDSON	59	601126
CEMP	TM B 6	SAMSONOV, G PADERN	59	300143
CPH	TM2O 3	PANKRATZ, L KING	63	202114
CPL	TRANSITION METALS	KAKUSHADZE, T	61	300818
CPL	TRANSITION METALS	WOLCOTT, N	55	601137
CRYS	TRANSITION METALS	DWIGHT, A	61	201200
MISC	TRANSITION METALS	WATT, G W	61	700590

REAC	TRANSITION METALS	AGEEV, N KOPETSKII	59	201230

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CRYS	U	SUTTON, A EELES, W	62	301600
PHAS	U	KLEMENT, W JAYARAM	63	301502
REAC	U	BESSONOV, A VLASOV	62	301188
BIB	U	ANON	58	601368
BIB	U	CROXTON, F	51	600955
BIB	U	ALLEN, R	53	600965
CEMP	U	RAUCH, E	56	601261
CEMP	U	HOLDEN, A	58	601562
CEMP	U	KATZ, J	58	601533
CEMP	U	RIVIERE, J	62	201805
CPH	U	MITKINA, E	59	201029
CPH	U	MOORE, G KELLEY, K	47	601646
CPH	U	GINNINGS, D CORRUC	47	601647
CPH	U	MORTH, J	56	600984
CPL	U	FLOTOW, H LOHR, H	60	601334
CPL	U	JONES, W M GORDON	52	400555
CPL	U	SMITH, P WOLCOTT	55	601137
CPL	U	GOODMAN, B HILLAIR	60	201518
CRYS	U	LUKESH, J	49	601652
CRYS	U	THEWLIS, J STEEPLE	54	601650
CRYS	U	WILSON, A RUNDLE	49	601657
CRYS	U	COOPER, A	62	601464
CRYS	U	JACOB, C WARREN, B	37	601653
CRYS	U	TUCKER, C	49	601371
CRYS	U	WILSON, A RUNDLE	49	601360
CRYS	U	STURCKEN, E POST	60	200857
CRYS	U	DAWSON, J	52	100187
CRYS	U	CHIOTTI, P KLEPFER	58	601074
CRYS	U	TUCKER, C	50	601176
CRYS	U	THEWLIS, J	52	100202
CRYS	U	THEWLIS, J	51	400569
CRYS	U	TUCKER, W SENIO, P	56	601016
CRYS	U	TUCKER, C SENIO, P	53	600964
CRYS	U	TUCKER, C SENIO, P	52	601251
CRYS	U	TUCKER, T	52	600673
CRYS	U	TUCKER, C W	52	400570
CRYS	U	TUCKER, C W	52	400571
CRYS	U	BRIDGE, J	56	601656
CRYS	U	CASH, A HUGHES, E	61	201362
CRYS	U	DONOHUE, J	61	201361
CRYS	U	LANIESSE, J ENGLAN	60	201980
CTEX	U	GOODMAN, M	60	601331
CTEX	U	SCHUCH, A F LAQUER	52	400568
CTEX	U	LEHV, P LANGERON	55	601005
CTEX	U	LLOYD, L	59	601203
DH	U	HOLLEY, C HUBER, E	60	601178
CTEX	U	BRIDGE, J	56	601656
DH	U	HUBER, E V HOLLEY	52	400565
DH	U	MOORE, G KELLEY, K	47	601646
ELCH	U	SMIRNOV, M SKIBA	61	300992
ERES	U	HOVL, J	56	601303
ERES	U	TYLER, W WILSON, A	53	100185
ERES	U	BERLINCOURT, T	59	601655
ERES	U	MURK, K	59	601523
ERES	U	DAHL, A VAN DUSEN	47	601644
MISC	U	KATZ, J J RABINOWI	51	400578
MPP	U	HOLDEN, A	58	601562
MPP	U	KATZ, J	58	601533
MPP	U	WATSON, J WILDER	60	201321
PHAS	U	THEWLIS, J	52	100202
PHAS	U	BUTCHER, B	56	601031
PHAS	U	ANON	56	601302
PHAS	U	KURODA, T SUZUKI	58	601326
PHAS	U	BLUMENTHAL, B	60	601342
PHAS	U	MUELLER, M HITHERM	62	601431
PHAS	U	ALLENDORFER, A	50	400539
PHAS	U	TUCKER, C W	52	400570
PHAS	U	LEHR, P LANGERON	57	601058
PHAS	U	DAHL, A I CLEAVES	49	400580
PHAS	U	FISHER, E	61	201270
PHAS	U	JOHNSON, R	61	201263
PHAS	U	ANON	56	601419
PHAS	U	ANON	57	601507
PHAS	U	BAUMRUCKER, J CHIS	53	601651

PHAS U	BUZZARD, R LISS, R	53	601649
PHAS U	CHRISTIAN, J	59	601621
PHAS U	FISHER, E	61	601455
PHAS U	KLEPFER, H	57	601506
PHAS U	SEMENCHENKOV, A	61	201894
REAC U	KATZ, J J RABINOWI	51	400578
REAC U	DEUTSCH, N ERVIN	60	500123
REAC U	BESSONOV, A VASLOV	61	201390
REAC U	DERGE, G MARTIN, A	44	201526
REV U	KAUFMANN, A	62	601429
REV U	NICHOLS, R	57	601102
REV U	HANTOS, R	58	601075
REV U	ANON	58	601539
REV U	ANON	58	601538
REV U	VETEJSKA, K	60	601199
REV U	CHISWICK, H DWIGHT	58	601207
SPK U	ELYASHEVICH, M	53	601413
SPK U	MOROZOVA, N STARTS	57	601416
SPK U	BOVEY, L ATHERTON	61	601422
SPK U	DIRINGER, M	60	601363
SPK U	ATHERTON, N BOVEY	60	601327
SPK U	SCHUURMANS, P	46	601290
SPK U	MCNALLY, J	52	100211
SPK U	MCNALLY, J	50	400523
SPK U	VAN DER BOSCH, J	49	400526
SPK U	VANDEN BOSCH, J C	50	400554
SPK U	SMITH, D D STOKENB	51	400564
SPK U	STRIGANOV, A KOROA	55	600989
SPK U	BEDREAG, O	54	601013
SPK U	OSARO, F PERLMAN	52	400572
SPK U	SMITH, D	52	601249
SPK U	BURKHART, L STUKEN	49	601373
SPK U	BAKULINCE, I IONOV	59	601135
SPK U	BOVEY, L WISE, H	59	601154
SPK U	ANON	58	601549
SPK U	ROGOSA, G SCHWARZ	53	500124
SPK U	NARBUTT, K LAPUTIN	62	201779
TCON U	MAKIN, B	54	601286
TCON U	WEEKS, J	55	601282
TCON U	WESTPHAL, R	55	601270
TCON U	ANON	57	601313
TCON U	FARIS, F	57	601310
TCON U	TYLER, W WILSON,A	53	100185
TRT U	AUBERT, H	62	201995
TCON U	SMITH, K	57	601063
TCON U	ERIKSEN, V HALG, W	55	600934
TCON U	DAYTON, R	58	601525
THER U	FLOTOW, H LOHR, H	60	601334
THER U	LEMMON, A WARD, J	52	601012
THER U	BREWER, L BROMLEY	47	400581
THER U	SCHICK, H ANTHROP	63	301579
THER U	MACWOOD, G	58	601143
THER U	ACKERMANN, R THORN	62	601616
THER U	MOORE, G KELLEY, K	47	601646
THER U	SKIDMORE, I MORRIS	62	601607
THER U	KENDALL, W	62	601684
TRT U	ALLENDORFER, A	50	400539
TRT U	DAHL, A I CLEAVES	49	400580
TRT U	FISHER, E	61	201270
TRT U	ANON	57	601507
TRT U	BURKE, J DIXON, P	62	301420
TRT U	DAHL,A VAN DUSEN	47	601644
VAP U	RAUH, E THORN, R	54	600948
VAP U	GILBREATH, J	52	601314
VAP U	GILBREATH, J	60	601333
VAP U	GILBREATH, J	57	601300
VAP U	GILBREATH, J	55	601274
VAP U	HANLIN, H	60	700951
VAP U	DEISS, W	62	300877
VAP U	RAUH, E THORN, R	54	601223
VAP U	ACKERMANN, R RAUH	62	601685
VAP U	ACKERMANN, R THORN	62	601616
CEMP U B 2	KLOPP, W	59	601542
CRYS U B 2	LUNSFORD, J FRIES	61	601466
CTEX U B 2	KLOPP, W	59	601542
CTEX U B 2	BECKMAN, G KIESSLI	56	601049
PHAS U B 2	HOWLETT, B	61	601357
THER U B 2	KLOPP, W	59	601542

CRYS	U B 4	STEPANOVA, A ZHURA	58	601111
CRYS	U B 4	ZALKIN, A TEMPELTO	53	100198
CTEX	U B 4	STEPANOVA, A ZHURA	58	601111
REV	U B 4	MATTERSON, K JONES	61	300324
CRYS	U B 12	BERAUT, F BLUM, P	49	601363
REAC	U B 12	PADERNO, Y	61	201276
PHAS	U BORIDES	BREWER, L SAWYER	50	601400
DF	U B SYST	ALCOCK, C GRIEVESO	62	601606
DH	U B SYST	ALCOCK, C GRIEVESO	62	601606
PHAS	U B SYST	HOWLETT, B	51	601357
PHAS	U B SYST	ANON	60	601328
PHAS	U B SYST	ALCOCK, C GRIEVESO	62	601606
THER	U B SYST	ALCOCK, C GRIEVESO	62	601606
PHAS	U B C SYST	TOTH, L	61	201256
PHAQ	U BE	BADAEVA, T KUZNETS	61	201833
PHAS	U BE C SYST	BRISI, C ABBATTIST	61	201507
DH	U BR	SHCHUKAREV, S VASI	58	200847
SPK	U BR SYST	PRIGENT, J	60	200934
BIB	U C	SEDDON, J	60	601380
CEMP	U C	HOPKINS, B	62	300516
CEMP	U C	KLOPP, W	59	601542
CPH	U C	WESTRUM, E	62	601689
CRYS	U C	WILLIAMS, J SAMBEL	60	601388
CRYS	U C	ATODA, T HIGASHI	61	301399
CRYS	U C	FERGUSON, I STREET	61	601418
CRYS	U C	CHIOTTI, P	52	601237
CRYS	U C	NOWOTNY, H	58	601079
CRYS	U C	CARTER, J H DAANE	51	400561
CRYS	U C	VOGEL, R KEMPTER	59	601177
CTEX	U C	KLOPP, W	59	601542
DH	U C	FARR, J HUBER, E	59	601200
ERES	U C	GRIFFITHS, L	62	201569
PHAS	U C	BRIGGS, G GUHA, J	62	301416
REAC	U C	MURBACH, E TURNER	62	202105
VAP	U C	VOZZELLA, P MILLER	62	202156
CPL	U C	COMBARIEU, A COSTA	63	202021
KIN	U C	ANTILL, J PEAKALL	59	200883
KIN	U C	CHUBB, W TOWNLEY	61	201311
MPP	U C	BOETTCHER, A SCHNI	60	601201
PHAS	U C	FERGUSON, I STREET	61	601418
PHAS	U C	NEWKIEK, H BATES	59	601165
REAC	U C	FARR, J HUBER, E	59	601200
REAC	U C	CARTER, J H DAANE	51	400561
REAC	U C	PEAKALL, K ANTILL	62	601682
REAC	U C	GREGOIRE, P	62	201488
REV	U C	SEDDON, J	60	601380
REV	U C	ROUGH, F CHUBB, W	60	600810
MPP	U C	BROWN, D STOBO, J	62	301198
CPL	U C	COMBARIEN, A COSTA	63	301206
THER	U C	GROSSMAN, L	63	301237
TCON	U C	EDWARDS, R	52	601235
THER	U C	FARR, J HUBER, E	59	601200
THER	U C	WESTRUM, E	62	601689
THER	U C	KLOPP, W	59	601542
TRT	U C	CHIOTTI, P	52	601237
TRT	U C	NEWKIEK, H BATES	59	601165
CRYS	U C 2	ATODA, T HIGASHI	61	301399
PHAS	U C 2	BRIGGS, G GUHA, J	62	301416
DH	U C 2	HUBER, E HEAD, E	63	202056
CEMP	U C 2	KLOPP, W	59	601542
CPH	U C 2	WESTRUM, E	62	601689
CRYS	U C 2	ATOJI, M MEDRUD, R	59	700867
CRYS	U C 2	FERGUSON, I STREET	61	601418
CRYS	U C 2	BREDIG, M	60	700852
CRYS	U C 2	GILLAM, E	62	601680
CTEX	U C 2	KLOPP, W	59	601542
DF	U C 2	FUJISHIRO, S	61	601440
PHAS	U C 2	FERGUSON, I	61	201139
PREP	U C 2	TAKADA, Y IMOTTO	61	201937
THER	U C 2	FUJISHIRO, S	61	601440
THER	U C 2	WESTRUM, E	62	601689
THER	U C 2	KLOPP, W	59	601542
VAP	U C 2	FUJISHIRO, S	61	601440
VAP	U C 2	LEITNAKER, J WITTE	62	300393
VAP	U C 2	EICK, H RAUH, E	62	601614
DH	U C 2	HUBER, E HEAD, E	63	301247
CPH	U C 2	LEVINSON, L	62	301292
CRYS	U 2C 3	GILLAM, E	62	601680

MPP	U 2C 3	MALLETT, M GERDS	61	100203
BIB	U CARBIDES	JONES, P	60	201004
CRYS	U CARBIDES	CHIOTTI, P	49	601416
MPP	U CARBIDES	BARNES, E MUNRO, W	57	601035
REAC	U CARBIDES	BARNES, E MUNRO, W	57	601035
REAC	U CARBIDES	WILHELM, H CHIOTTI	49	400536
THER	U CARBIDES	BREWER, L BROMLEY	47	400581
TRT	U CARBIDES	CHIOTTI, P	49	601416
SPK	U COMPOUNDS	DUNN, H	56	601024
REAC	U COMPOUNDS	KATZ, S	62	201971
SPK	U COMPOUNDS	EDING, H CARR, E	61	201061
BIB	U C SYST	BOWMAN, F	60	601346
BIB	U C SYST	COMSTOCK, M	60	600623
CRYS	U C SYST	AUSTIN, A	59	601120
CPH	U C SYST	MUKAIBO, T NAITO	62	601610
CRYS	U C SYST	RUNDLE, R WILSON	58	601112
DF	U C SYST	ALCOCK, C GRIEVESO	62	601606
DH	U C SYST	ALCOCK, C GRIEVESO	62	601606
MPP	U C SYST	CHUBB, W DICKERSON	62	601481
PHAS	U C SYST	ANON	57	601298
PHAS	U C SYST	ANON	53	601311
CRYS	U C SYST	SHARMA, B	63	301194
THER	U C SYST	CUNNINGHAM, G WARD	63	301208
PHAS	U C SYST	ANON	57	601507
PHAS	U C SYST	ANON	53	601513
PHAS	U C SYST	ANON	57	601516
PHAS	U C SYST	ANON	57	601555
PHAS	U C SYST	ANON	57	601559
PHAS	U C SYST	CHUBB, W PHILLIPS	61	601442
PHAS	U C SYST	WILLIAMS, J SAMBEL	59	200872
PHAS	U C SYST	ANON	59	601349
PHAS	U C SYST	SILVERMAN, L	50	601364
PHAS	U C SYST	ANON	60	601414
PHAS	U C SYST	WILHELM, E	56	601264
PHAS	U C SYST	RUNDLE, R WILSON	58	601112
PHAS	U C SYST	WILSON, W	60	601193
PHAS	U C SYST	MALLETT, M GERDS	52	100188
PHAS	U C SYST	BLUMENTHAL, B	56	601044
PHAS	U C SYST	ALCOCK, C GRIEVESO	62	601606
PHAS	U C SYST	BLUMENTHAL, B	59	601692
PHAS	U C SYST	EPREMIUM, E	57	601516
REAC	U C SYST	SIVARTS, E	57	601109
REAC	U C SYST	LOCK, L GAMBINO, J	56	601015
REAC	U C SYST	CARTER, J H DAANE	50	400560
THER	U C SYST	ANON	60	601414
THER	U C SYST	BREWER, L BROMLEY	58	601145
THER	U C SYST	ALCOCK, C GRIEVESO	62	601606
THER	U C SYST	HULLEY, C	63	601690
MPP	U C O SYST	NAMBA, S IMOTA, S	61	400611
REAC	U C O SYST	TRACHENKO, E VLASO	63	301605
PHAS	U CE SYST	SAVITSKII, E BARON	62	201552
SPK	U CL4	WING, R	61	201127
SPK	U CL2O SYST	WING, R	61	201127
REAC	U F	NGHI, N	61	201687
REAC	U F	STEVENSON, J RUEHL	53	201727
CPL	U F 4	BURNS, J OSBORNE	60	200848
DH	U F 4	MALTSEV, V	60	201161
PHAS	U F 4	KIRSHENBAUM, A	61	201183
REAC	U F 4	CAVELL, R CLARK, H	62	201725
SPK	U F 4	RAMBIDI, N AKISHIN	61	300763
THER	U F 4	GALKIN, N	61	201248
VAP	U F 4	AKISHIN, P KHODEEV	61	300453
THER	U F 6	PARKS, B BARTON, D	60	200884
REV	U F 6	TSUJIMURA, S	62	201986
REAC	U F SYST	RESHETNIKOV, F GUR	62	300972
DH	U FE SYST	AKHACHINSKIY, V KO	62	301104
THER	U HALIDES	BREWER, L BROMLEY	47	400581
THER	U HALIDES	MACWOOD, G	58	601143
PHAS	U HF C SYST	RUDY, E BENESOVSKY	63	301333
ERES	U MN	HAMAGUCHI, Y KUNIT	62	201568
PHAS	U MO	KAWASAKI, M NAGASA	60	201491
REAC	U MO	BELLOT, J DOSIER	58	201627
PHAS	U MO SYST	TANGRI, K WILLIAMS	61	201308
PHAS	U MO SYST	KRAMER, D RHODES	61	201367
PHAS	U MO SYST	IVANOV, O BADAEVA	61	201868
PHAS	U MO SYST	IVANOV, O SEMENCHE	61	201896
PHAS	U MO C	RUDY, E BENESOVSKY	63	301566
PHAS	U MO C SYST	RUDY, E BENESOVSKY	63	301332

PHAS	U MO C SYST	FIZZOTTI, C SARAC	62	201697
PHAS	U MO CR SYST	BADAEVA, T KUZNETS	61	201899
SPK	U MO X6	HORTON, J THOMAS	62	201851
PHAS	U MO ZR SYST	IVANOV, O BAGROV	61	201840
PHAS	U MO ZR SYST	IVANOV, O BAGROV	61	201898
BIB	U N	COMSTOCK, M	60	600623
BIB	U N	KERR, W	62	601461
CEMP	U N	KLOPP, W	59	601542
CRYS	U N	KELLER, D	61	601445
CRYS	U N	CHIOTTI, P	52	601237
CRYS	U N	MUELLER, H KNOTT	58	601136
CRYS	U N	ANON	59	601550
CTEX	U N	KELLER, D	61	601445
CTEX	U N	KEMPTER, C ELLIOTT	59	601150
CTEX	U N	KLOPP, W	59	601542
DH	U N	GROSS, P HAYMAN, C	62	601621
ERES	U N	KELLER, D	61	601432
PHAS	U N	NEWKIEK, H BATES	59	601165
PHAS	U N	BRIGGS, G GUHA J	62	301416
REAC	U N	NEWTON, A S JOHNSO	51	400559
REV	U N	KERR, W	62	601461
TCON	U N	KELLER, D	61	601432
TCON	U N	EDWARDS, R	52	601235
THER	U N	KLOPP, W	59	601542
TRT	U N	OLSON, M MULFORD	63	301546
TRT	U N	CHIOTTI, P	52	601237
TRT	U N	NEWKIEK, H BATES	59	601165
VAP	U N	OLSON, M MULFORD	63	301546
REAC	U N 2	BESSONOV, A VLASOV	62	201942
CRYS	U 2N 3	EVANS, P	62	601463
DH	U 2N 3	GROSS, P HAYMAN, C	62	601621
CRYS	U NITRIDES	CHIOTTI, P	49	601177
THER	U NITRIDES	BREWER, L BROMLEY	47	400581
TRT	U NITRIDES	CHIOTTI, P	49	601177
CRYS	U N SYST	DAYTON, R	57	601509
DH	U N SYST	MOREAU, C PHILIPPO	61	201313
MPP	U N SYST	RUNDLE, R BAENZIGE	59	601140
PHAS	U N SYST	WILLIAMS, J SAMBEL	59	200872
PHAS	U N SYST	RUNDLE, R BAENZIGE	48	601375

PHAS	U N SYST	VAUGHAN, D	56	601004
PHAS	U N SYST	DAYTON, R	57	601509
REAC	U N SYST	RUNDLE, R BAENZIGE	59	601140
SPK	U N SYST	VAUGHAN, D	56	601004
THER	U N SYST	BREWER, L BROMLEY	58	601145
PHAS	U N C SYST	AUSTIN, A GERDS, A	58	601117
PHAS	U NB	NORTON, J OGILVIE	59	201811
PHAS	U NB SYST	IVANOV, O TEREKHOV	61	201945
CEMP	U NB SYST	BATES, L BARNARD	61	201202
PHAS	U NB C SYST	RUDY, E BENESOVSKY	63	301333
PHAS	U NB MO SYST	IVANOV, O TEREHKON	61	201832
PHAS	U NB MO SYST	IVANOV, O TEREHKOV	61	201841
PHAS	U NB MO SYST	IVANOV, O TEREHKOV	61	201842
CEMP	U O	ZHUKOVSKII, V VASL	62	201982
CRYS	U O	YOUNG, W LYNDS, L	62	201567
DF	U O	MARKIN, T BONES, R	62	201819
KIN	U O	BESSONOV, A ALASOV	62	201964
KIN	U O	VOLPE, M MIHAILOVI	62	201919
MSP	U O	DEMAUA, G BURNS, R	60	601163
PHAS	U O	SUDO, K KIGOSHI, A	61	201530
PHAS	U O	ALEXANDER, C	62	201921
PHAS	U O	RUEDORFF, N KEMMLE	62	201776
REAC	U O	POLUNINA, G KOVBA	61	201624
REAC	U O	SAND, T IMOTO, S	60	200963
REAC	U O	UKAJI R MINAMI, F	61	201623
REAC	U O	ANTH , J	62	201973
THER	U O	SCHICK, H ANTHROP	63	301579
CRZS	U O 2	WILLIS, B	63	301623
REAC	U O 2	ORBACH, H	62	301547
THER	U O 2	SCHICK, H ANTHROP	63	301579
TRT	U O 2	CHIKALLA, T	63	301203
TRT	U O 2	MUMPTON, F ROY, R	60	301308
REAC	U O 2	CORDFUNKE, E	61	201785
VAP	U O 2	GERDANIAN, P DODE	62	201886
BIB	U O 2	REISWIG, R	61	601378
BIB	U O 2	WENSRICH, C	60	700972
BIB	U O 2	BELLE, V	57	601511
BIB	U O 2	SHAPIRO, Z	57	601512
BIB	U O 2	HAUSNER, H	59	601530

CPH	U O 2	KOENIG, N	58	601366
CPH	U O 2	CABBAGE, A WELCH	61	601443
CPH	U O 2	POPOV, M GALCHENKO	58	601153
CPL	U O 2	JONES, W M GORDON	52	400555
CPL	U O 2	OSBORNE, D WESTRUM	53	600988
CRYS	U O 2	HASHIGUCHI, R MATS	60	200856
CRYS	U O 2	TUXWORTH, R	60	600849
CRYS	U O 2	CHIOTTI, P	49	601416
CRYS	U O 2	VAN ARKEL, A	24	701056
CRYS	U O 2	CHIOTTI, P	52	601237
CRYS	U O 2	ROBINS, R WILKS, R	62	201821
CTEX	U O 2	LAMBERTSON, W	56	601323
CTEX	U O 2	FUIKERSON, S	60	60136[illegible]
CTEX	U O 2	KOENIG, N	58	601366
CTEX	U O 2	KEMPTER, C ELLIOTT	59	601150
CTEX	U O 2	HALDEN, F WOHLERS	59	201836
DH	U O 2	ACKERMANN, R	56	601322
DH	U O 2	ARONSON, S	61	201318
DF	U O 2	ACKERMANN, R THORN	58	601510
ELCH	U O 2	LAMBERTSON, W	56	601323
KIN	U O 2	ARONSON, S ROOF, R	57	601068
KIN	U O 2	KUHLMAN, C	48	201904
KIN	U O 2	KUHLMAN, C	48	201115
MISC	U O 2	BUTLER, G HAUSNER	60	200915
MPP	U O 2	KOENIG, N	58	601366
MPP	U O 2	PRIEST, H PRIEST	58	601147
MSP	U O 2	DEMAUA, G BURNS, R	60	601163
PHAS	U O 2	KOENIG, N	58	601366
PHAS	U O 2	LAMBERTSON, W	56	601323
PHAS	U O 2	HERING, H PERIO, P	52	601236
PHAS	U O 2	PERIO, P	53	601216
PHAS	U O 2	BARD, R BOWERSOX	57	601060
PHAS	U O 2	NEWKIEK, H BATES	59	601165
PHAS	U O 2	ROTHWELL, E	62	601476
PHAS	U O 2	EVANS, P	61	201362
PHAS	U O 2	COHEN, I SCHANER	62	201845
REAC	U O 2	BARD, R BOWERSOX	57	601060
REAC	U O 2	ARONSON, S ROOF, R	57	601068
REAC	U O 2	BLACKBURN, P WEISS	58	601114
REAC	U O 2	ANDERSON, J SAWYER	60	601172
REAC	U O 2	HOEKSTRA, H	61	201177
REAC	U O 2	DAS, C SAHOO, B	61	201466
REAC	U O 2	LYNDS, L	62	201682
REV	U O 2	KAUFMANN, A	62	601429
REV	U O 2	SEDDON, J	60	601380
REV	U O 2	SHAPIRO, E	57	601296
REV	U O 2	BELLE, J	58	601202
REV	U O 2	TENNERY, J	59	601535
RHO	U O 2	KOENIG, N	58	601366
S	U O 2	ACKERMANN, R	56	601322
TCON	U O 2	ROSE, R	58	601392
TCON	U O 2	DAYTON, R	58	601527
TCON	U O 2	DAYTON, R	58	601526
TCON	U O 2	DAYTON, R	58	601529
TCON	U O 2	DAYTON, R	58	601557
TCON	U O 2	DAYTON, R	58	601556
TCON	U O 2	REISWIG, R	61	601378
TCON	U O 2	KOENIG, N	58	601366
TCON	U O 2	HEDGE, J	57	601294
TCON	U O 2	MAKIN, B	54	601286
TCON	U O 2	GILBREATH, J	56	601274
TCON	U O 2	FLINTA, J	58	601095
TCON	U O 2	BETHOUX, O THOMAS	61	201534
TCON	U O 2	BERG, K FLINTA, L	58	201533
TCON	U O 2	SCOTT, R	58	601115
TCON	U O 2	POWERS, R	60	201184
TCON	U O 2	BERG, K	58	601544
TCON	U O 2	ROSS, A	58	601493
TCON	U O 2	TENNERY, J	59	601535
THER	U O 2	ACKERMANN, R	56	601273
THER	U O 2	ACKERMANN, R THORN	58	601087
THER	U O 2	ACKERMANN, R GILLE	58	601233
THER	U O 2	ARONSON, S BELLE	58	601077
THER	U O 2	ACKERMANN, R GILLE	56	601045
THER	U O 2	SMIRNOV, M	60	201191
THER	U O 2	IVANOV, V KRUGLYKH	62	601604
TRT	U O 2	CHIOTTI, P	52	601237
TRT	U O 2	CHIOTTI, P	49	601416

TRT	U O 2	WISNYI, L	57	601500
VAP	U O 2	ACKERMANN, R	56	601322
VAP	U O 2	ACKERMANN, R	55	601273
VAP	U O 2	ACKERMANN, R THORN	58	601510
VAP	U O 2	ANON	57	601514
VAP	U O 2	IVANOV, V KRUGLYKH	62	601604
TRT	U O 2	WISNYI, L PIJANOWS	57	601081
TRT	U O 2	ANDERSON, J SAWYER	60	601172
TRT	U O 2	NEWKIEK, H BATES	59	601165
ZKP	U O 2	SMIRNOV, M	60	201191
CPH	U O 3	POPOV, M GALCHENKO	58	601153
CPL	U O 3	JONES, W M GORDON	62	400555
CRYS	U O 3	CORNMAN, W	62	301030
CRYS	U O 3	DEWOLFF, P	61	601424
CRYS	U O 3	CONNOLLY, D	59	601365
CRYS	U O 3	WAIT, E	55	601268
DF	U O 3	ACKERMANN, A THORN	60	601174
KIN	U O 3	STREKALOVSKII, V A	61	201079
KIN	U O 3	KUHLMAN, C	48	201105
KIN	U O 3	KUHLMAN, C	48	201904
MPP	U O 3	PRIEST, H PRIEST	58	601147
REAC	U O 3	VLASOV, G ZHUKOVSK	62	301612
SPK	U O 3	TSUBOI, M TERADA	62	201721
MSP	U O 3	DEMAUA, G BURNS, R	60	601163
REAC	U O 3	VLASOV, V SHALAGIN	61	201027
REAC	U O 3	STREKALOVSKII, V A	61	201079
REAC	U O 3	MURAI, M EYRAUD, C	62	201692
SPK	U O 3	BOROVSKI, I BARINO	50	400551
TRT	U O 4	WISNYI, L PIJANOWS	57	601056
REAC	U 20 5	KHLEBNIKOV, G SIMA	61	201625
CRYS	U 30 5	SIEGEL, S	55	601267
CPL	U 30 7	WESTRUM, E GRONVOL	62	300752
DH	U 30 7	MUKAIBO, T NAITO	62	601609
THER	U 30 7	MUKAIBO, T NAITO	62	601609
CPH	U 30 8	KHOMYAKOV, K SPITS	61	300729
CPH	U 30 8	POPOV, M GALCHENKO	58	601153
CPH	U 30 8	ZAJIC, V	60	601170
CPH	U 30 8	POWERS, H WELCH, F	61	601444
CPL	U 30 8	WESTRUM, E	58	601553
CRYS	U 30 8	CHODURA, B MALY, J	58	601546
CRYS	U 30 8	GRONVOLD, F	48	601379
CRYS	U 30 8	ANDERSON, A	58	601078
CRYS	U 30 8	WILSON, W	60	601183
CPL	U 30 8	WESTRUM, E GRONVOL	59	601133
DH	U 30 8	POPOV, M IVANOV, M	57	601086
DHT	U 30 8	KHOMYAKOV, K SPITS	61	300729
ERES	U 30 8	BRIDGMAN, P	51	400533
PHAS	U 30 8	PERIO, P	53	601216
PHAS	U 30 8	HERING, H PERIO, P	52	601236
REAC	U 30 8	KHLEBNIKOV, G SIMA	61	201625
REAC	U 30 8	VLASOV, V KOZLOV	62	201591
THER	U 30 8	WESTRUM, E	58	601553
CPL	U 40 9	OSBORNE, D	56	601254
CRYS	U 40 9	BELBEOCH, B PIEKAR	60	601426
REAC	U 40 9	HOEKSTRA, H	61	201177
THER	U 40 9	OSBORNE, D	56	601254
TRT	U 40 9	ZHUKOVSKII, E TKAC	63	301628
CEMP	U OXIDES	WILLARDSON, R MOOD	58	601104
CRYS	U OXIDES	MAKAROV, E	61	301114
CRYS	U OXIDES	FRIED, S	56	601021
DHD	U OXIDES	VLASOV, V LEBEDEV	61	201185
KIN	U OXIDES	VLASOV, V LEBEDEV	61	201185
KIN	U OXIDES	BESSONOV, A VASLOV	61	201468
PHAS	U OXIDES	BUD' KOV, T TRESVY	59	201395
THER	U OXIDES	BREWER, L BROMLEY	47	400581
REAC	U OXIDES	MANDELBERG, C	61	201335
BIB	U O SYST	LANG, S	53	100195
BIB	U O SYST	COMSTOCK, M	60	600623
CRYS	U O SYST	BOULLE, A JARY, R	49	400537
CRYS	U O SYST	BAINZIGER, N WILSO	58	601142
DF	U O SYST	BLACKBURN, P	58	601113
ERES	U O SYST	BRABERS, M	58	601212
MPP	U O SYST	CLAZTON, J ARONSON	58	601122
PHAS	U O SYST	GERDANIAN, P DODE	62	300355
PHAS	U O SYST	GRONVOLD, F	55	601001
PHAS	U O SYST	HOEKSTRA, H SIEGEL	58	601209
PHAS	U O SYST	KATZ, J	51	400534
PHAS	U O SYST	HOEKSTRA, R SIEGEL	56	601022

PHAS	U O SYST		
	HOEKSTRA, H	55	601280
BIB	U O SYST		
	MANDIL, I SCOTT, R	61	201303
ERES	U O SYST		
	HAUFFE, K	41	601483
DH	U O SYST		
	BURDESE, A	58	601560
KIN	U O SYST		
	LEIBOWITZ, L	61	201314
PHAS	U O SYST		
	AUKRUST, E FOERLAN	62	601605
PHAS	U O SYST		
	MARKIN, T ROBERTS	62	601608
PHAS	U O SYST		
	WESTRUM, E GRONVOL	62	601613
PHAS	U O SYST		
	SCHANER, B	60	601686
PHAS	U O SYST		
	WILSON, W	61	601448
PHAS	U O SYST		
	HOEKSTRA, H	58	601487
PHAS	U O SYST		
	KIUKKOLA, K	62	601469
TCON	U O SYST		
	BRUBERS, M	58	601546
TCON	U O SYST		
	ROSS, A	58	601493
THER	U O SYST		
	ACKERMAN G, R THORN	62	601616
THER	U O SYST		
	MARKIN, T ROBERTS	62	601608
THER	U O SYST		
	WESTRUM, E GRONVOL	62	601613
THER	U O SYST		
	KIUKKOLA, K	62	601469
VAP	U O SYST		
	ACKERMANN, R THORN	62	601616
VAP	U O SYST		
	WESTRUM, E GRONVOL	62	601613
VAP	U O SYST		
	CHAPMAN, A	63	202016
PHAS	U O SYST		
	PERIO, P	53	601283
PHAS	U O SYST		
	MILLER, C MERTEN	61	601407
PHAS	U O SYST		
	BARON, J	61	601433
PHAS	U O SYST		
	ROBERTS, L	61	601434
PHAS	U O SYST		
	BRIGHT, N	56	601288
PHAS	U O SYST		
	STEEB, S	60	200882
PHAS	U O SYST		
	BOULLE, A JARY, R	49	400537
PHAS	U O SYST		
	ALBERMAN, K ANDERS	49	400538
PHAS	U O SYST		
	STREKALOVSKIY, V B	61	400613
PHAS	U O SYST		
	BLACKBURN, P	58	601113
PHAS	U O SYST		
	PERIO, P	55	601033
PHAS	U O SYST		
	BAINZIGER, N WILSO	58	601142
REV	U O SYST		
	BAGLEY, K OLIVER	59	601141
SPK	U O SYST		
	GRONVOLD, F	56	601001
THER	U O SYST		
	HOEKSTRA, R SIEGEL	56	601022
THER	U O SYST		
	WAGNER, C	56	601025
THER	U O SYST		
	BREWER, L BROMLEY	58	601146
VAP	U O SYST		
	ALEXANDER, C	62	300533
DH	U O CL SYST		
	SHCHUKAREV, S VASI	58	200798
KIN	U Y O SYST		
	FELTEN, E AITKEN	62	201690
CRYS	U RE2		
	HATT, B	61	200929
DH	U SI		
	GROSS, P HAYMAN, C	62	601621
DH	U SI2		
	GROSS, P HAYMAN, C	62	601621
DH	U SI3		
	GROSS, P HAYMAN, C	62	601621
DH	U 3SI2		
	GROSS, P HAYMAN, C	62	601621
PHAS	U TA C SYST		
	RUDY, E BENESOVSKY	63	301333
PHAS	U TH C SYST		
	BENESOVSKY, F RUDY	61	300542
PHAS	U W C		
	RUDY, E BENESOVSKY	62	201628
REAC	U W O		
	TRUNOV, V LOVBA, L	61	201486
PHAS	U ZR SYST		
	BENESOVSKY, E RUDY	61	100181
PHAS	U ZR SYST		
	BOROVSKII, I MARCH	60	201014
PHAS	U ZR		
	ZEGLER, S	62	201647
PHAS	U ZR C SYST		
	RUDY, E BENESOVSKY	63	301333
PHAS	U ZR NB SYST		
	IVANOV, O GOMOZOV	61	201895
PHAS	U ZR O SYST		
	GEBHARDT, E ELSSNE	61	301049

V

CPH	V		
	JOHNSON, R	60	301488
CPH	V		
	GOLUTOIN, Y KOZLOV	62	301458
CPL	V		
	HENDRICKS, J RISER	63	301239
MPP	V		
	LINCOLN, R ASAI, G	62	301525
VAP	V		
	SAXER, R	63	301576
THER	V		
	KUBASCHEWSKI, O	62	601577
MISC	V		
	GAIDUKOV, G GAIDUK	62	301139
BIB	V		
	WOHLL, M	60	700723
CEMP	V		
	RICKERT, E BECKETT	49	601638
CEMP	V		
	BURGER, J TAYLOR	61	600853
CPL	V		
	KREBS, K	63	202082
CPL	V		
	SHIMIZU, M TAKAHAS	63	202135
COPT	V		
	GOLDSMITH, A HIRSC	60	700930
CPH	V		
	FIELDHOUSE, I LANG	60	601583
KIN	V		
	KUBASCHEWSKI, O	62	601577
CPH	V		
	GOLDSMITH, A HIRSC	60	700930
CPH	V		
	JOSHI, S MITRA, S	60	200767
CPH	V		
	GOLUTVIN, Y KOZLOV	62	301093
CPL	V		
	CLARK, C	62	601563

CPL	V	CLUSIUS, K FRANZOS	60	700987
CPL	V	JOSHI, S MITRA, S	60	200767
CPL	V	BIEGANSKI, Z STALI	61	700660
CPL	V	BOORSE, H BERMAN	55	700887
CRYS	V	JAMES, W	61	201196
CTEX	V	JAMES, W	61	201196
CTEX	V	FIELDHOUSE, I LANG	60	601583
ERES	V	TAYLOR, M LLEWELL	62	201675
ERES	V	GOLDSMITH, A HIRSC	60	700930
H	V	GOLDSMITH, A HIRSC	60	700930
MPP	V	RICKERT, E BECKETT	49	601638
MPP	V	BRADFORD, S	61	300368
PMCH	V	BOLEF, D	61	200936
PHAS	V	SEYBOLT, A	4P	601484
PHAS	V	ZELIKMAN, A KISLYA	61	701037
PHAS	V	SAVITSKII, E BARON	62	300609
PHAS	V	BRADFORD, S	61	300368
PHAS	V	KOMJATHY, S	61	201434
PHAS	V	KOMJATHY, S READ	60	201394
REAC	V	DEUTSCH, N ERVIN	60	600123
REAC	V	BLOCK, F FERRANTE	61	201013
REAC	V	KORNILOV, I MATVEY	61	400588
REV	V	ZELIKMAN, A KISLYA	61	701037
REV	V	SPERNER, X	61	300372
REV	V	KORNILOV, I MATVEE	62	201946
S	V	CLUSIUS, K FRANZOS	60	700987
SPK	V	ROSENZWEIG, N PORT	60	700996
SPK	V	MURAKAWA, K KAMEI	53	601218
SPK	V	ROSENZWEIG, N PORT	60	700901
SPK	V	BOLOTIN, G VOLOSHI	62	201830
TCON	V	FIELDHOUSE, I LANG	60	601583
TCON	V	GOLDSMITH, A HIRSC	60	700930
THEO	V	ROSENZWEIG, N PORT	60	700901
THEO	V	ROSENZWEIG, N PORT	60	700996
THER	V	SCHICK, H ANTHROP	63	300994
THER	V	BIEGANSKI, Z STALI	61	700660
VAP	V	HANLIN, H	60	700951
REV	VAPOR PRESSURE	RABINOVICH, I	62	300975
THEO	VAPORIZATION	SEARCY, A SCHULZ	63	300980
THEO	VAPORIZATION	SALTER, L	63	300986
THEO	VAPORIZATION	VERHAEGEN, G STAFF	62	301010
THEO	VAPORIZATION	NEUMANN, K VOLKER	32	900212
THEO	VAPORIZATION	ROSENBLATT, G	63	301562
THEO	VAPORIZATION	ACKERMANN, R THORN	62	301391
THEO	VAPORIZATION	FEUER, P	63	202031
REV	VAPORIZATION	FISHTINE, Q	63	202032
THEO	VAPORIZATION	KOLLAR, G PROSZT	63	202076
THEO	VAPORIZATION	PUTILOV, K MELMICH	62	300602
THEO	VAPORIZATION	FIRSOVA, L	62	300697
THEO	VAPORIZATION	REIMANN, C	62	300469
THER	V B	MEERSON, G	60	300298
CRYS	V 3B 2	KIEFFER, B BENESOV	58	600619
DH	V BR3	VASILKOVA, I	61	201222
REAC	V BR3	SHCHUKAREV, S TOLM	62	201809
CEMP	V C	MATSKEVICH, T KAZA	62	300952
CEMP	V C	NOGUCHI, S SATE, T	60	300227
CPH	V C	NEEL, D PEARS, C	61	300146
DF	V C	ALEKSEEVA V I	61	300201
DHD	V C	BITTNER, H GORETZK	62	301132
MPP	V C	NORTON, J MOWRY, A	49	300157
PHAS	V C	NORTON, J	60	701001
S	V C	KAUFMAN, L	62	300910
SPK	V C	PARKINSON, W NICHO	59	00612
THER	V C	FUJISHIRO, S	62	6 11477
THER	V C	ANON	60	700992
THER	V C	ANON	60	700904
VAP	V C	ANON	60	700992
VAP	V C	ANON	60	700904
VAP	V C	FUJISHIRO, S	60	300463
VAP	V C	ANON	60	600666
CEMP	V C	BITTNER, H GORETZK	62	202004
MPP	V C	GIORGI, A SZELARZ	63	202039
REAC	V C	SAMSONOV, G		301571
DH	V 2C	ALEKSEEV, V SHVART	60	600909
PHAS	V CARBIDES	ALYAMOVSKII, S GEL	61	201374
MPP	V C SYST	SAVOSTIANOVA, N A	60	300204
DF	V C SYST	ALEKSEEVA, V SHVAR	61	700632
MPP	V C SYST	BURYLEV, B	61	301071

PHAS	V C SYST	STORMS, E MCNEAL	62	300608
PHAS	V C SYST	SAVOSTIANOVA, N	60	300204
ERES	V CR	TAYLOR, M LLEWELL	62	201675
PHAS	V C FE SYST	BELIKOV, A SAVINSK	62	300863
PHAS	V MN	WATERSTRAT, R	62	201584
PHAS	V MO SI SYST	SAVITSKII, E BARON	62	201798
MPP	V N	SAMSONOV, G VERKHO	62	300997
MPP	V N	SAMSONOV, G VERKHO	61	301573
S	V N	KAUFMAN, L	62	300910
ZKP	V N	KOROLEV, L MOROZOV	62	301272
THER	V N	KOROLEV, L MOROZOV	63	301273
THEO	V N	BAUGHAN, E	59	300866
CRYS	V N 2	HAHN, H	61	701046
PHAS	V N 2	HAHN, H	61	701046
DH	V NITRIDES	SAMSONOV, G	60	700947
CEMP	V NITRIDES	SAMSONOV, G	60	700947
REV	V NITRIDES	SAMSONOV, G	60	700947
CRYS	V O	MAGNELI, A	60	600617
THER	V O	HOCH, M	61	301475
SPK	V O	ORTENBERG, F	61	300821
SPK	V O	NICHOLLS, R	62	300698
SPK	V O	LAGERQVIST, A SELI	57	300166
SPK	V O	NICHOLLS, R	62	601625
SPK	V O	BERG, R A SINANOGL	60	300177
REAC	V O	MARGOTIN, P STUCKE	61	201574
SPK	V O	PRASAD, S	63	202120
OPK	V O	LAGERQVIST, A	57	301290
CRYS	V O	POPOV, YU	62	301321
SPK	V O	LAGERQVIST, A	57	600885
SPK	V O	KEENAN, P SCHROEDE	52	600911
SPK	V O	TAWDE, N MURTHY, N	57	600913
THER	V O 2	SCHICK, H ANTHROP	63	301580
CRYS	V O 2	HECKINGBOTTOM, R L	62	300704
MPP	V O 2	DAY, J FREYMANN, M	49	400517
PHAS	V O 2	WESTMAN, S	61	700545
SPK	V O 5	CONLON, D DOYLE, W	61	201325
REAC	V 2O 3	GELD, P MATVEENKO	62	201913
REAC	V 2O 3	MATSOURA, R	61	201028
CRYS	V 2O 5	BACHMAN, H	60	200795
REAC	V 2O 5	MATSOURA, R	61	201028
REAC	V 2O 5	DEDUIT, J	61	700611
DH	V 2O 5	KING,E KOEHLER	62	301500
ERES	V 2O 5	BOROS, J	61	301192
REAC	V 2O 5	HAGENMULLER, P LES	63	301467
VAP	V 2O 5	NEUGENAUER, J	63	301311
ERES	V 2O 5	MANAKOV, P ESIN, O	62	202096
CRYS	V 2O 5	BACHMANN, H	61	201154
CRYS	V 3O 5	ASBRINK, S FRIBERG	59	200825
SURF	V OXIDES	LEPINSKIKH, B	60	201215
PHAS	V OXIDES	ANDERSSON, S	59	201178
CRYS	V OXIDES	MAGNELI, A ANDERSO	61	201566
PHAS	V O SYST	WESTMAN, S	63	301621
THEO	V O SYST	GELD, P TSKHAI, V	63	202036
CPH	V O SYST	YAKOVLEVA, M KRASI	61	300351
CRYS	V O SYST	ARIYA, S POPOV, Y	62	300599
DF	V O SYST	MAH, A KELLEY, K	61	300407
DH	V O SYST	MOROZOVA, M P EGER	60	300247
DH	V O SYST	MAH, A KELLEY, K	61	300407
KIN	V O SYST	CUBICCIOTTI, D	52	100194
MPP	V O SYST	BOGDANOVA, N LOGIN	62	300640
PHAS	V O SYST	KUBASCHEWSKI, O	62	601577
PHAS	V O SYST	BURDESE, A BORLERA	60	200945
PHAS	V O SYST	NADOR, B	60	200938
VAP	V O SYST	SHCHUKAREV, S SEME	59	301353
PHAS	V O SYST	KOSUGE, K TAKADALI	62	301276
CRYS	V O SYST	GELD, P TSKHAY, V	63	301225
PHAS	V O SYST	ANON	60	701015
PHAS	V O SYST	GELD, P V ALYAMOSK	61	300200
PHAS	V O SYST	WESTMAN,S NORDMAR	60	201329
VAP	V O SYST	ANON	60	701015
ZKP	V O SYST	ARIYA, S MOROZOVA	62	300600
REAC	V O C SYST	GELD, P MATVEYENKOL	62	301224
PHAS	V RE SYST	TYLKINA, M POVAROV	60	201291
DH	V SI SYST	GOLUTVIN, Y	62	301229
CPH	V SI SYST	GOLUTVIN, Y KOZLOV	62	300568
PHAS	V W SYST	RUDY, E BENESOVSKY	62	300630
THER	V X	SHCHUKAREV, S TOLM	62	201540
THER	V CL O	NAGARAJAN, G	62	201816

THER	V CL O SYST	NAGARAJAN, G	62	201772
CPH	V 3SI	PANKRATZ, L KELLEY	63	301319
REAC	V X SYST	ARADI, A VITANYI	61	201862

W

REAC	W	BROPHY, J KREIDER	63	202011
SPK	W	CLAUS, H ULMER, K	63	202017
MPP	W	KOPETSKIY, CH	62	301270
THER	W	KRAFTMAKHER, YA	62	301280
BIB	W	GOODWIN, T	56	601547
BIB	W	WOHLL, M	60	700723
BIB	W	WENSRICH, C	60	700972
BIB	W	RICHERT, E BECKETT	49	700564
CEMP	W	GUMENYUK, V LEBEDE	61	700553
COPT	W	COFFMAN, J COULSON	61	701040
CPH	W	HOCH, M	61	201167
CPH	W	CHEKHOVSKOY, V SHU	62	300868
CPH	W	JOHNSON, R	60	301488
CPH	W	KIRILLIN, V SHEIND	62	300638
CPH	W	KIRILLIN, V SHEIND	62	300687
CPH	W	KIRILLIN, V SHEIND	62	300360
CPH	W	KIRILLIN, V SHEIND	62	300531
CPH	W	RUDKIN, R PARKER	60	600614
CPH	W	JAEGER, F ROSENBOH	27	700506
CPH	W	JAEGER, F ROSENBOH	30	700505
CPH	W	FORSYTHE, W WORTHI	25	700507
CPH	W	ZWIKKER, C SCHMIDT	28	700515
CPH	W	MAGNUS, A DANZ, H	26	700560
CPH	W	BRONSON, H CHISHOL	33	700561
CPH	W	MAGNUS, A HOLZMANN	29	700562
CPH	W	HOCH, M JOHNSTON	61	700613
CPL	W	CLARK, C	62	601563
CPL	W	FEATHERSTON, F NEI	63	301444
CPL	W	MYERS, A	60	700981
CPL	W	LANGE, F	24	700563
CPL	W	SHARAN, B	61	301070
CRYS	W	COFFMAN, J COULSON	61	701040
CRYS	W	UMANSKII, M ZUBENK	60	600859
CRYS	W	ANDERSON, S	60	200845
CRYS	W	KOMAR, A SHREDNIK	62	300695
CRYS	W	GETTE, E FOOTE, F	35	700510
CRYS	W	LU S CHANG, Y	41	700512
CRYS	W	CHAULTON, M DAVIS	55	700513
CRYS	W	MATYUSHENKO, N	62	301150
CTEX	W	NOWOTNY, H LAUBE	61	600844
DF	W	COFFMAN, J COULSON	61	701040
ERES	W	BRIDGMAN, P	51	400533
ERES	W	TYE, R	61	201117
ERES	W	GUMENYUK, V LEBEDE	61	700553
KIN	W	ONG, J	62	201536
KIN	W	ARZHANYI, P VOLKOV	62	201975
KIN	W	GULBRANSEN, E ANDR	62	201770
MISC	W	HAMPEL, C	61	200889
MISC	W	BASKIN, M TRETYAKO	62	201951
MPP	W	ARGENT, B MILNE, G	60	201039
PHAS	W	ZALABAK, C	61	701026
PHAS	W	SHAFFER, P	61	700941
PHAS	W	COFFMAN, J COULSON	61	701040
PHAS	W	BRILLIANTOV, N STA	61	300807
PHAS	W	HAWORTH, C	60	201017
PHAS	W	OREHOTSKY, J STEIN	62	300519
PHAS	W	CHAULTON, M DAVIS	55	700513
PHAS	W	ROSTOKER, W	60	201396
PHAS	W	FUNKE, V NOVIKOVA	62	201704
REAC	W	KUBASCHEWSKI, O HO	60	201038
REAC	W	BECKER, J BECKER	61	201091
REAC	W	GULBRONSEN, E ANDR	59	600638
REAC	W	DEUTSCH, N ERVIN	60	500123
REAC	W	FRANTSEVICH, I LAV	59	200869
REAC	W	KOMAR, A TALANIN	60	200843
REAC	W	MITROFANOV, O	62	301097
REAC	W	ZELIKMAN, A KREIN	62	201861
REV	W	WOHLL, M	60	701053
REV	W	SMITHELLS, C	53	700509
REV	W	RICHERT, E BECKETT	49	700564
REV	W	SYRE, R	61	201579
SPK	W	ALLEN, R GLASIER	60	200828

SPK	W	LARRABEE, A	57	201223
SPK	W	ROSENZWEIG, N PORT	60	700996
SPK	W	ROSENZWEIG, N PORT	60	700901
SPK	W	MOORE, C	58	601088
SPK	W	BODMER, A	54	600936
TCON	W	TYE, R	61	201117
TCON	W	GUMENYUK, V LEBEDE	61	700553
THEO	W	ROSENZWEIG, N PORT	60	700996
THEO	W	ROSENZWEIG, N PORT	60	700901
TKER	W	GOODWIN, T	56	601547
THER	W	RUDKIN, R PARKER	60	600614
TRT	W	ZALABAK, C	61	200988
TRT	W	OREHOTSKY, J STEIN	62	300519
TRT	W	TAYLOR, A RYDEN, H	62	301027
VAP	W	NELSON, L KUEBLER	63	301540
VAP	W	CANO, G	62	301423
VAP	W	LANGMUIR, I	13	700504
VAP	W	COFFMAN, J COULSON	61	701040
VAP	W	ZWIKKER, C	26	700508
H	W B	MEZAKI, R TILLEUX	62	601617
S	W B	MEZAKI, R TILLEUX	62	601617
THER	W B	LEITNAKER, J BOWMA	62	300553
PHAS	W B 4	CHRETIEN, A HELGOR	61	201084
H	W 2B	MEZAKI, R TILLEUX	62	601617
S	W 2B	MEZAKI, R TILLEUX	62	601617
H	W 2B 5	MEZAKI, R TILLEUX	62	601617
S	W 2B 5	MEZAKI, R TILLEUX	62	601617
REAC	W BORIDES	SAMSONOV, G	59	500120
REAC	W B SYST	SAMSONOV, G STRASH	62	300990
REAC	W BR3	MCCARLEY, R BROWN	62	201856
DH	W BROMIDES	SHCHUKAREV, S KOKO	60	201159
CEMP	W C	ZUBENKO, Y SOKOLSK	62	201676
COPT	W,C	COFFMAN, J COULSON	61	701040
THER	W C	ALKESEEV, V SHARTS	63	301168
VAP	W C	FESENKO, V BOLGAR	63	301216
CRYS	W C	GORELIK, C ELYUTIN	62	301230
CPH	W C	NEEL, D PEARS, C	61	300146
CRYS	W C	LECIEJWICZ, J	61	201199
CRYS	W C	COFFMAN, J COULSON	61	701040
CRYS	W C	BUTORINA, L	60	700986
CRYS	W C	PARTHE, E SADAGOPA	62	300520
DF	W C	COFFMAN, J COULSON	61	701040
DF	W C	GLEISER, M CHIPMAN	62	300886
MPP	W C	KOVALCHENKO, M SAM	62	300920
PHAS	W C	COFFMAN, J COULSON	61	701040
PHAS	W C	GOLDSCHMIDT, H BRA	63	301457
PHAS	W C	NADLER, M KEMPTER	60	300301
PHAS	W C	FORELIK, C YELYUTI	62	300884
REAC	W C	SHVEIKIN, G	62	301588
REV	W C	LECIEJWICZ, J	61	201199
THER	W C	SCHICK, H ANTHROP	63	301579
THER	W C	COFFMAN, J COULSON	60	701006
VAP	W C	COFFMAN, J COULSON	61	701040
VAP	W C	COFFMAN, J COULSON	60	701006
THER	W 2C	SCHICK, H ANTHROP	63	301579
BIB	W COMPOUNDS	GODFREY, L BELL, P	59	600607
THER	W C SYST	CUNNINGHAM, G WARD	63	301208
PHAS	W C SYST	ORTON, G	61	300510
PHAS	W C SYST	SARA, R DOLLOFF, R	62	601622
PHAS	W C SYST	GOLDSCHMIDT, H BRA	62	601626
REAC	W C SYST	SAMSONOV, G STRASH	62	300990
THER	W CL	SHCHUKAREV, S NOVI	59	200800
MPP	W C N SYST	GERASIMOV, A KONEV	61	300511
PHAS	W HF SYST	GIESSEN, B RUMP, I	62	201433
PHAS	W HF	SELL, H KEITH, G	61	201860
PHAS	W MO RE SYST	TYLKINA, M POVAROV	60	201292
CRYS	W N	KHITROVA, V PINSKE	59	201620
CRYS	W N	KHITROVA, V PINSKE	60	201619
CEMP	W NITRIDES	SAMSONOV, G	60	700947
CRYS	W NITRIDES	KHITROVA, V PIN		301110
DH	W NITRIDES	SAMSONOV, G	60	700947
REV	W NITRIDES	SAMSONOV, G	60	700947
EMF	W O	GERASIMOV, Y VASIL	60	200925
MSP	W O	DEMAUA, G BURNS, R	60	601163
VAP	W O	GLEMSER, O HAESELE	62	201927
REAC	W O	ANDES, G HECKEL, R	62	201498
REAC	W O	AUSTIN, L	61	201387
SPK	W O	VITTALACHAR, U KRI	64	600897

DH	W M 2		
GERASIMOV, Y VASIL		60	600657
DF	W O 2		
GERASIMOV, Y VASIL		60	600657
VAP	W O 2		
NEUGENAUER, J		63	301311
EMF	W O 2		
GERASIMOV, Y VASIL		60	700999
MSP	W O 2		
DEMAUA, G BURNS, R		60	601163
REAC	W O 2		
KOZMANOV, Y		60	201005
S	W O 2		
GERASIMOV, Y VASIL		60	700999
THER	W O 2		
GERASIMOV, Y VASIL		60	700999
CRYS	W O 3		
GRAHAM, J WADSLEY		61	201026
CRYS	W O 3		
TANISAKI, S		60	201077
DF	W O 3		
ACKERMANN, R THORN		58	601510
DF	W O 3		
ACKERMANN, A THORN		60	601174
MSP	W O 3		
DEMAUA, G BURNS, R		60	601163
PHAS	W O 3		
TANISAKI, S		60	201076
SPK	W O 3		
HEGEDUS, A		61	201144
THER	W O 3		
HEGEDUS, A		61	201144
THER	W O 3		
VASILEVA, I GERASI		60	200965
THER	W O 3		
ACKERMAN., R THORN		58	601087
TRT	W O 3		
TANISAKI, S		60	201076
VAP	W O 3		
ACKERMANN, R THORN		58	601510
CPH	W OXIDES		
KING, E WELLER, W		60	700973
CPL	W OXIDES		
KING, E WELLER, W		60	700973
CRYS	W OXIDES		
OZEROV, R		55	701064
DHT	W OXIDES		
KING, E WELLER, W		60	700973
KIN	W OXIDES		
BLACKBURN, P ANDRE		60	601582
PHAS	W OXIDES		
KING, E WELLER, W		60	700973
REAC	W OXIDES		
PERKINS, R CROOKS		61	201090
REAC	W OXIDES		
HAMAMURA, T		60	201386
S	W OXIDES		
KING, E WELLER, W		60	700973
THER	W OXIDES		
BLACKBURN, P ANDRE		60	601582
THER	W OXIDES		
KING, E WELLER, W		60	700973
VAP	W OXIDES		
BATTLES, J STPIERR		61	300310
EMF	W O SYST		
GERASIMOV, I VASIL		62	300755
PHAS	W O SYST		
ANON		60	701015
PHAS	W O SYST		
BATTLES, J EBIHARA			300853
PHAS	W O SYST		
ST PIERRE, G EBIHA		62	300547
REAC	W O SYST		
SPEISER, R		60	600861
PHAS	W O SYST		
KOUBA, L TRUNOV, V		62	301278
PHAS	W O SYST		
BERGER, I SEVASTY		56	301186
THER	W O SYST		
BATTLES, J EBIHARA			300853
THER	W O SYST		
GERASIMOV, I VASIL		62	300755
THER	W O SYST		
KSENOFONTOVA, R VA		62	301388
VAP	W O SYST		
ANON		60	701015
VAP	W O SYST		
BLACKBURN, P		62	300543
KIN	W O SYST		
GULBRANSEN, E		63	301465
REAC	W O C SYST		
HEGEDUS, A GADO, P		60	200788
PHAS	W OS SYST		
TAYLOR, A		61	201206
PHAS	W PD SYST		
TYLKINA, M POLYAKO		61	700623
PHAS	W RE SYST		
SAVITSKII, E TYLKI		59	201281
REAC	W RE		
KOZMANOV, Y FESHCH		61	201589
REAC	W REFRACTORIES		
MAY, C HOEKSTRA, P		61	700863
PHAS	W TI C SYST		
VATOLIN, N KISLING		62	301008
PHAS	W V		
RUDY, E BENESOVSKY		62	300630

Y

VAP	Y		
NESMEYANOV, AN PRI		62	301310
CEMP	Y		
MICHAELSON, H		50	400529
CPL	Y		
MONTGOMERY, H PELL		61	601447
CPL	Y		
GOODMAN, B		52	100208
CPL	Y		
JENNINGS, L MILLER		60	201049
CPL	Y		
LEBEDEV, V		48	700702
CRYS	Y		
LUNDIN, C KLODT, D		60	601346
CRYS	Y		
SPEDDING, F DAANE		56	700703
CRYS	Y		
HERRMANN, K DAANE		56	700905
CRYS	Y		
FOUTFELKER, R SIET		62	701089
CTEX	Y		
MEYERHOFF, R SMITH		62	300809
DG	Y		
HUBER, E		57	601316
DH	Y		
HUBER, E HEAD, E		57	601059
ERES	Y		
ANON		58	601524
ERES	Y		
GOODMAN, B		52	100208
ERES	Y		
HALL, P LEGVOLD, S		59	601164
H	Y		
KELLEY, K		60	700891
MPP	Y		
ANON		61	500131
MPP	Y		
BERNSTEIN, B SMITH		59	700807
MPP	Y		
HABERMANN, C DAANE		63	301466
PMCH	Y		
SMITH, J CARLSON		57	700746
PMCH	Y		
SMITH, J GJEVRE, J		60	700812

REAC	Y		
SIMMONS C FUNSTON		61	700808
REAC	Y		
NOLTING, H SIMMONS		60	700841
REAC	Y		
THOMPSON, A HOTTON		26	700828
REV	Y		
LOVE, B		60	700735
S	Y		
KELLEY, K		60	700891
SPK	Y		
SCHWARZSCHILD, M		57	601047
SPK	Y		
ROSENZWEIG, N PORT		60	700996
SPK	Y		
SHADMI, Y		61	700964
SPK	Y		
GARSTANG, R		52	100207
SPK	Y		
CATALAN, M RICO, F		57	601206
SPK	Y		
MOORE, C		52	100201
SPK	Y		
MOORE, C		52	100200
SPK	Y		
BUSCOMBE, W MERRIL		52	100199
REV	Y		
STRUAT, K WEIK, H		60	601167
REV	Y		
VICKERY, R		60	601173
SPK	Y		
BOHM VITENSE, E		60	601169
SPK	Y		
DIETER, V EHRENSTE		57	601100
SPK	Y		
MERRILL, P GREENST		58	601097
SPK	Y		
TESKE, R		56	601043
SPK	Y		
SKINNER, H		55	700761
SPK	Y		
CATALAN, M RICO, F		52	601250
SPK	Y		
CATALAN, M RICO, F		52	700800
SPK	Y		
BOVEY, F		56	700825
THEO	Y		
ROSENZWEIG, N PORT		60	700996
THER	Y		
SCHICK, H ANTHROP		63	300994
THER	Y		
SPEDDING, F FLYNN		64	700824
TRT	Y		
HABERMANN, C DAANE		63	301466
VAP	Y		
BEAVIS, L		60	701016
VAP	Y		
KARELIN, V NESMEYA		62	700701
VAP	Y		
MCKENZIE, D JENKIN		60	700806
VAP	Y		
KARELIN, R NESMEYA		62	300914
VAP	Y		
BAUGHAN, E		54	700809
VAP	Y		
ACKERMANN, R RAUH		62	700840
VAP	Y		
ACKERMANN, J RAUH		62	700909
THER	Y +		
VASILEV, V ZOLOTAR		59	700823
CEMP	Y B 2		
JOHNSON, R DAANE		63	301489
CRYS	Y B 4		
BINDER, I		60	700830
PHAS	Y B 4		
BINDER, I		56	700816
CEMP	Y B 6		
BENOIT, R		55	700820
CRYS	Y B 6		
BERTAUT, F BLUM, P		52	700813
CRYS	Y B 6		
FISCHER HJALMARS, I		54	700821
CRYS	Y B 6		
KUDINTSEVA, G POLY		58	700737
CRYS	Y B 6		
BINDER, I		60	700830
PHAS	Y B 6		
KUDINTSEVA, G POLY		58	700737
PHAS	Y B 6		
TVOROGOV, N		59	700831
PHAS	Y B 12		
BINDER, I LAPLACA		59	700818
CRYS	Y B 12		
LAPLACA, S BINDER		61	700802
CRYS	Y B SYST		
BINDERS, L		56	601269
PHAS	Y B SYST		
BINDER, I		56	700816
CTEX	Y C		
SAMSONOV, G MAKARE		61	700811
MPP	Y C		
SAMSONOV, G KOSOLA		62	700743
PHAS	Y C		
SAMSONOV, G MAKARE		61	700811
CRYS	Y C 2		
ATOJI, M		61	700810
CRYS	Y C 2		
ATOJI, M		61	700864
CRYS	Y 2C 3		
SPEDDING, F GSCHNE		58	700834
DH	Y CL3		
SPEDDING, F FLYNN		54	700822
DH	Y CL3		
MONTGOMERY, R HUBE		60	700833
PHAS	Y GROUP 5A		
LUNDIN, C KLODT, D		62	201630
PHAS	Y GROUP IVA		
LUNDIN, C KLODT, D		62	201582
THER	Y ION		
VASILEV, V ZOLOTAR		59	700823
PHAS	Y LA O SYST		
CASSEDANNE, J FORE		61	700801
PHAS	Y MG		
MYKLEBUST, R DAANE		62	201580
CRYS	Y N		
KEMPTER, C KRIKORI		57	700837
CRYS	Y N		
KEMPTER, C		57	601295
CRYS	Y N		
LUNDIN, C KLODT, D		60	601346
THER	Y N		
KUBASHEVSKI, O EVA		56	700829
DHD	Y O		
WALSH, P WHITE, D		58	700806
F	Y O		
BREWER, L CHARDRAS		59	700721
H	Y O		
KELLEY, K		60	700891
S	Y O		
KELLEY, K		60	700891
SPK	Y O		
ORTENBERG, F		61	300821
SPK	Y O		
MERRILL, P GREENST		56	601007
SPK	Y O		
TESKE, R		56	601043
SPK	Y O		
UHLER, U AKERLIND		61	300476
VAP	Y O		
SCHICK, H ANTHROP		63	300994
CPH	Y 2O 3		
PANKRATZ, L KING		62	300958
CPH	Y 2O 3		
GOLDSTEIN, H NGILS		59	601198
CPH	Y 2O 3		
NILSON, F PETTERSO		60	700819

CPH	Y 2O 3	CURTIS, C	57	700836
CPL	Y 2O 3	GOLDSTEIN, H	58	601551
CPL	Y 2O 3	GOLDSTEIN, H NEILS	59	700836
CRYS	Y 2O 3	STARITZKY, E	56	601292
CRYS	Y 2O 3	FERT, A	62	301447
CRYS	Y 2O 3	CURTIS, C	57	700836
DH	Y 2O 3	MONTGOMERY, R HUBE	60	700833
DH	Y 2O 3	HUBER, E HEAD, E	57	700842
H	Y 2O 3	KELLEY, K	60	700891
MPP	Y 2O 3	CURTIS, C THARP, A	59	700804
MPP	Y 2O 3	CURTIS, C	57	700836
PHAS	Y 2O 3	FANG, F KUZNETSOV	62	301443
PHAS	Y 2O 3	TOROPOV, N GALAKHO	61	201966
PHAS	Y 2O 3	STARITZKY, E	56	601030
S	Y 2O 3	KELLEY, K	60	700891
SPK	Y 2O 3	UHLER, U AKERLIND	59	700844
SPK	Y 2O 3	WICKERSHEIM, K LEF	61	201301
THER	Y 2O 3	KUBASHEVSKI, O EVA	56	700829
VAP	Y 2O 3	WALSH, P WHITE, D	58	700806
VAP	Y 2O 3	WALSH, P GOLDSTEIN	60	700814
VAP	Y 2O 3	MOTT, W	18	700827
PHAS	Y RE	LOVE, B	60	201699
PHAS	Y U O SYST	CHASE, G	62	201826
CPL	YB	LOUNASMAA,O	63	301527
DH	YB	SAVAGE, W HUDSON	59	601126
DH	YB	HUBER, E	56	601291
DH	YB	HUBER, E HEAD, E	56	601041
SPK	YB	KREBS, K NELKOWSKI	56	601029
SPK	YB	BURBRIDGE, E BURBR	55	601003
SPK	YB	MERRILL, P GREENST	56	601007
SPK	YB	BODMER, A	54	600936
SPK	YB	BRIX, P	52	400566
VAP	YB	ANON	56	601319
VAP	YB	SAVAGE, W HUDSON	59	601126
CEMP	YB B 6	SAMSONOV, G PADERN	59	300143
CRYS	YB B 6	STEPANOVA, A ZHURA	58	601111
CTEX	YB B 6	STEPANOVA, A ZHURA	58	601111
CRYS	YB N	EICK, H BAENZIGER	56	601046
ERES	YB N	DIDCHENKO, R GORTS	63	301435
PHAS	YB N	EICK, H BAENZIGER	56	601046
REAC	YB N	EICK, H BAENZIGER	56	601046
REAC	YB NITRIDES	EICK, H	57	601053
CPH	YB2O 3	PANKRATZ, L KING	63	202114
CPL	YB2O 3	JUSTICE, B WESTRUM	63	300907
DH	YB2O 3	HUBER, E	56	601291
REAC	YB OXIDES	EICK, H	57	601053
PHAS	YB TH	GSCHNEIDER, K	62	201700

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ERES	ZN	RENUCCI, L LANGERO	61	201517
REV	ZN	GIUORD, J	62	201554
BIB	ZR	ANON	61	701047
BIB	ZR	FELDMAN, M	61	701045
BIB	ZR	WILLIAMS, G BAKER	52	600904
CPH	ZR	CARTER, W	61	601631
CPH	ZR	FIELDHOUSE, I LANG	60	601583
CPL	ZR	MYERS, A	60	700981
CPL	ZR	BORELIUS, G	60	601168
CPL	ZR	KNEIP, G BETTERTON	61	201412
CRYS	ZR	BYKOV, V KAZARNIKO	59	201649
CRYS	ZR	LAWLEY, A	60	200801
CRYS	ZR	FELDMAN, M	61	701045
PHAS	ZR	RICHTER, H WINCIERZ	62	201766
THER	ZR	KUBASCHEWSKI, O	62	601677
CRYS	ZR	FOUNFELKER, R SIET	62	701089
CTEX	ZR	CARTER, W	61	601631
CTEX	ZR	NOWOTNY, H LAUBE	61	600844
CTEX	ZR	FIELDHOUSE, I LANG	60	601583
DH	ZR	FEDOROV, G	60	600823
DHT	ZR	HERTZRICKEN, S SLY	62	300708
ERES	ZR	BERLINCOURT, T	59	601655
ERES	ZR	BRIDGMAN, P	51	400533
ERES	ZR	POWELL, R H TYE, R	61	700653
MISC	ZR	SPACEK, V	61	200888
MISC	ZR	SPINK, D	61	200891
MPP	ZR	SKINNER, G BECKETT	50	601225
CRYS	ZR	JAMIESON, J	63	301253

CPL	ZR	KNIEF, G BETTERTON	63	301264
MPP	ZR	RILEY, W MCCLELLAN	62	301080
PHAS	ZR	KORNILOV, I	60	200907
PHAS	ZR	FELDMAN, M	61	701045
PHAS	ZR	IANNIELLO, L	61	201146
PHAS	ZR	WORNER, H	60	200991
PHAS	ZR	BIBB, A BEARD, A	61	201344
PHAS	ZR	BEREZHNOI, A KORDY	62	201553
PHAS	ZR	NISHIHARA, M	60	201493
PHAS	ZR	WYDER, W HOCH, M	62	201581
PHAS	ZR	MANNAS, D SMITH, J	62	201786
PHAS	ZR	SEMENCHENKOV, A	61	201694
REAC	ZR	MIYAMOTO, O NAKASH	58	500118
REAC	ZR	BAKER, W	61	201057
REAC	ZR	ANDREEVA, V ALEKSE	62	201814
REV	ZR	SPERNER, F	61	300371
REV	ZR	OSTBERG, G	61	201364
SPK	ZR	RUBESKA, I	62	500119
SPK	ZR	ROSENZWEIG, N PORT	60	700996
SPK	ZR	SHADMI, Y	61	700954
SPK	ZR	SWEENEY, W SEAL, R	61	201112
SPK	ZR	SUWA, S	52	400575
SPK	ZR	NORRIS, J	60	601194
SPK	ZR	SHAW, C	55	600908
SURF	ZR	BLITON, J RECHTER	63	301133
TCON	ZR	TOIRELIKOV, V KOM	61	301101
TCMN	ZR	FIELDHOUSE, I LANG	60	601583
TCON	ZR	LOWRIE, R	61	700943
TCON	ZR	POWELL, R H TYE, R	61	700653
THEO	ZR	ROSENZWEIG, N PORT	60	700996
THER	ZR	SCHICK, H ANTHROP	63	300994
THER	ZR	FEDEROV, G SMIRNOV	61	601659
THER	ZR	CARTER, W	61	601631
THER	ZR	CARTER, W	62	300749
TRT	ZR	JAYARAMAN, A KLEME	63	301482
TRT	ZR	WILLIAMS, D JACKSO	62	301016
VAP	ZR	TOIRELNIKOV, V KOM	61	301101
VAP	ZR	YEMELYANOV, V	62	301626
VAP	ZR	FEDEROV, G SMIRNOV	62	601620
CPH	ZR	DOUGLAS, T	63	202029
MPP	ZR	KAREV, V KLYUCHARE	63	202064
TRT	ZR	ULY, J LAM, D IAN	61	202149
ZKP	ZR	SMIRNOV, M KOMAROV	60	201056
CRYS	ZR B 2	RUDY, E	61	201255
DF	ZR B 2	WARD, J ALEXANDER	61	701055
DH	ZR B 2	LOWRIE, R GRIST, R	61	300412
CRYS	ZR B 2	GORELIK, C ELYUTIN	62	301230
VAP	ZR B 2	KIBLER, G LYON, T	63	301259
THER	ZR B 2	LITTLE, A	62	301526
DH	ZR B 2	EPELBAUM, V A STAR	55	300194
H	ZR B 2	MEZAKI, R TILLEUX	62	601617
MPP	ZR B 2	SHCHERBAKOV, V VEY	60	300984
PHAS	ZR B 2	FORELIK, C YELYUTI	62	300884
PHAS	ZR B 2	MARTIN, R SEAGLE	61	300308
PHAS	ZR B 2	FUNKE, V IUDKOVSKI	63	301138
S	ZR B 2	MEZAKI, R TILLEUX	62	601617
SPK	ZR B 2	LOWRIE, R	62	601596
THER	ZR B 2	MEERSON, G	60	300298
THER	ZR B 2	BOLGAR, A	61	700938
THER	ZR B 2	LEITNAKER, J BOWMA	62	300392
TRT	ZR B 2	MARTIN, R SEAGLE	61	300308
VAP	ZR B 2	BOLGAR, A	61	700938
VAP	ZR B 2	LEITNAKER, J BOWMA	62	300392
VAP	ZR B 2	KIBLER, G LYON, T	61	300409
MPP	ZR B 2	MALYUCHKOV, O POVI	62	202095
MPP	ZR B 2	SHAFFER, P	62	202133
MPP	ZR B 2	TYRRELL, M HOUCK	63	202148
VAP	ZR B 2	LOWRIE, R	62	701081
VAP	ZR B 2	LOWRIE, R SCHOMCHE	62	300940
VAP	ZR B 2	SCHICK, H ANTHROP	63	300994
VAP	ZR B 2	ANON	62	601597
VAP	ZR B 2	LOWRIE, R	62	601596
VAP	ZR B 2	LOWRIE, R GRIST, R	61	300412
PHAS	ZR B SYST	ANON	60	701015
VAP	ZR B SYST	ANON	60	701015
PHAS	ZR B C SYST	NOWOTNY, H	61	201147
PHAS	ZR B C SYST	NOWOTNY, H RUDY, E	60	201799
PHAS	ZR B CR SYST	KOVALCHENKO, M SAM	60	300216

PHAS	ZR B2 MO SYST	KOVALCHENKO, M S	61	300193
PHAS	ZR B2 MO SYST	KOVALCHENKO, M SAM	60	300216
PHAS	ZR B N SYST	NOWOTNY, H RUDY, E	60	201799
PHAS	ZR B N SYST	RUDY, E BENESOVSKY	61	300486
CEMP	ZR BORIDES	SAMSONOV, G KISLYY	61	900200
EMF	ZR BORIDES	BECK, W	61	300477
REAC	ZR BORIDES	SAMSONOV, G	59	600120
DH	ZR BR4	TURNBULL, A	61	300259
CEMP	ZR C	HODDAD, R GOLDWATE	49	300159
CEMP	ZR C	HOPKINS, B ROSS, K	62	300515
REAC	ZR C	BARTLETT, R WADSWO	63	301183
VAP	ZR C	FESENKO, V BOLGAR	63	301216
CEMP	ZR C	INGOLD, J	63	301251
CTEX	ZR C	KRIKORIAN, WALLA	63	301285
DH	ZR C	MAH, A BOYLE, B	55	301297
CEMP	ZR C	BONDARENKO, B ERMA	62	301409
COPT	ZR C	COFFMAN, J COULSON	61	701040
COPT	ZR C	HODDAD, R E GOLDWA	49	300159
CPH	ZR C	FINCH, R	61	700547
CPL	ZR C	FINCH, R	61	700547
CRYS	ZR C	VAN ARKEL, A	24	701056
CRYS	ZR C	COFFMAN, J COULSON	61	701040
DF	ZR C	VIDALE, G	61	301610
REAC	ZR C	SAMSONOV, G		301571
THER	ZR C	LITTLE, A	62	301526
TRT	ZR C	SHAFFER, P	63	202132
CEMP	ZR C	BITTNER, H GORETZK	62	202004
MPP	ZR C	DERGUNOVA, V KOLON	63	202026
TRT	ZR C	GROSSMAN, L	63	202044
CRYS	ZR C	BENESOVSKY, F RUDY	60	700974
DF	ZR C	COFFMAN, J COULSON	61	701040
DHD	ZR C	BITTNER, H GORETZK	62	301132
ERES	ZR C	FINCH, R	61	700547
MPP	ZR C	NORTON, J MOWRY, A	49	300157
PHAS	ZR C	SHAFFER, P	61	701057
PHAS	ZR C	NORTON, J	60	701001
PKAS	ZR C	SHAFFER, P	61	700941
PHAS	ZR C	BENESOVSKY, F RUDY	60	700974
PHAS	ZR C	COFFMAN, J COULSON	61	701040
S	ZR C	KAUFMAN, L	62	300910
SPK	ZR C	COFFMAN, J KIBLER	60	700993
SURF	ZR C	HODDAD, R E GOLDWA	49	300169
TCON	ZR C	TAYLOR, R	62	300694
THER	ZR C	COFFMAN, J COULSON	60	701006
THER	ZR C	COFFMAN, J KIBLER	60	700993
THER	ZR C	BOLGAR, A	61	700936
THER	ZR C	ANON	60	700992
THER	ZR C	POLLOCK, B	61	600674
THER	ZR C	ANON	62	601597
THER	ZR C	ANON	60	700904
VAP	ZR C	VIDALE, G	61	301611
VAP	ZR C	SCHICK, H ANTHROP	63	300994
VAP	ZR C	ANON	60	700904
VAP	ZR C	ANON	60	700992
VAP	ZR C	BOLGAR, A	61	700938
VAP	ZR C	COFFMAN, J COULSON	60	701006
VAP	ZR C	COFFMAN, J KIBLER	60	700993
VAP	ZR C	COFFMAN, J COULSON	61	701040
VAP	ZR C	POLLOCK, B	61	600674
VAP	ZR C	COFFMAN, J COULSON	61	300293
VAP	ZR C	ANON	60	600666
THER	ZR C SYST	CUNNINGHAM, G WARD	63	301206
PHAS	ZR C SYST	BENESOVSKY, F RUDY	60	600648
PHAS	ZR C SYST	SARA, R DOLLOFF, R	62	301057
REAC	ZR C SYST	PORTNOI, K LEVINSK	61	300215
PHAS	ZR C SYST	SARA, R DOLLOFF, R	62	601622
VAP	ZR C SYST	POLLOCK, B D	61	700536
PHAS	ZR CA O SYST	GODINA, N KELER, E	61	201336
SPK	ZR CL4	BUCHLER, A BERKOWI	61	300183
VAP	ZR CL4	EVSTYUKHIN, A BARI	60	300882
THER	ZR CL SYST	RUZINOV, L BELOV		301568
PHAS	ZR CO	BAILEY, D SMITH, J	61	201646
PHAS	ZR CO O SYST	NEVITT, M DOWNEY	61	201267
MPP	ZR CR B SYST	MEYERSON, G	59	301115
VAP	ZR COMPOUNDS	ANON	61	300239
REV	ZR COMPOUNDS	BUDNIKOV, P CHEREP	63	301419
MPP	ZR COMPOUNDS	STRELETS, V PITAK	62	300624
CPH	ZR F 4	MCDONALD, R SINKE,	62	300662

DH	ZR F 4	GREENBERG, E SETTL	61	300199
DH	ZR F 4	SMITH, D MILLER, W	62	201542
DHT	ZR F 4	MCDONALD, R SINKE	62	300662
SPK	ZR F 4	BUCHLER, A BERKOWI	61	300183
SPK	ZR HALIDES	BUCHLER, A	60	201465
THER	ZR HALIDES	LUNGU, S	62	300736
PHAS	ZR HF SI SYST	SCHOB, O NOWOTNY	61	201547
PHAS	ZR HF X	NISELSON, L	62	201551
DH	ZR I 4	TURNBULL, A	61	300259
THER	ZR I 4	ALEKSANDROVSKAYA, A	62	201610
PHAS	ZR MG O SYST	GODINA, N KELER, E	61	201336
VAP	ZR N	FESENKO, V BOLGAR	63	301216
CRYS	ZR N	VAN ARKEL, A	24	701056
MPP	ZR N	SAMSONOV, G VERKHO	61	301573
VAP	ZR N	AKISHIN, P KHODEEV	62	300592
CEMP	ZR N	SAMSONOV, G FOMENK	63	202128
THEO	ZR N	BAUGHAN, E	59	300866
S	ZR N	KAUFMAN, L	62	300910
VAP	ZR N	KIBLER, G LYON, T	61	601579
VAP	ZR N	KIBLER, G LYON, T	61	601575
VAP	ZR N	KIBLER, G LYON, T	62	300427
CRYS	ZR N	LOWRIE, R	60	701014
MPP	ZR N	SAMSONOV, G VERKHO	62	300997
DF	ZR N	SMAGINA, Y KUTSEV	59	300345
CEMP	ZR NITRIDES	SAMSONOV, G	60	700947
DH	ZR NITRIDES	SAMSONOV, G	60	700947
REV	ZR NITRIDES	SAMSONOV, G	60	700947
CRYS	ZR N SYST	GROZIER, J	61	701018
KIN	ZR NB	COX, B CHADD, P	62	201963
PHAS	ZR NB SYST	LUNDEN, U E COX, R	61	300240
PHAS	ZR NB SYST	LUNDIN, C	59	201119
PHAS	ZR NI O SYST	NEVITT, M DOWNEY	61	201267
SPK	ZR O	DEUTSCH, A MERRILL	59	202027
CRYS	ZR O	FLODMARK, S	61	301033
DF	ZR O	ACKERMANN, R THORN	58	601510
DHD	ZR O	NAZIMOVA, N	60	201227
KIN	ZR O	AKRAM, K SMELTZER	62	201872
KIN	ZR O	DEBUIGNE, J LEHR	62	201886
PHAS	ZR O	KORNILOV, I	60	200769
REAC	ZR O	SENSE	62	201588
SPK	ZR O	MURTHY, N	62	601623
SPK	ZR O	ROSEN, B	62	301560
SPK	ZR O	ORTENBERG, F	61	300821
SPK	ZR O	KIESS, C	48	600685
SPK	ZR O	AFAF, M	50	600914
THEO	ZR O	FLODMARK, S	61	301033
THER	ZR O	SCHICK, H ANTHROP	63	301579
THER	ZR O	ACKERMANN, R THORN	58	601087
THER	ZR O	BEREZHNOI, A	62	201541
VAP	ZR O	ACKERMANN, R THORN	58	601510
CPH	ZR O 2	ROBIJN, P	63	301568
CPH	ZR O 2	VICTOR, A DOUGLAS	60	700949
CRYS	ZR O 2	TEUFER, G	62	301604
ERES	ZR O 2	COCCO, A BARBARIOL	62	301430
ERES	ZR O 2	DIXON, J LAGRANGE	63	301436
MPP	ZR O 2	POLUBOYARINOV, D G	62	301552
CPH	ZR O 2	VICTOR, A DOUGLAS	60	202153
TRT	ZR O 2	VISHNEVSKII, I	62	202154
TRT	ZR O 2	WOLTEN, G	63	202161
PHAS	ZR O 2	FANG, F KUZNETSOV	62	301443
PHAS	ZR O 2	HINZ, I DIETZEL, A	62	301472
PHAS	ZR O 2	PEREZ Y JORBA, M	62	301491
PHAS	ZR O 2	KELER, E ANDREEVA	63	301496
PHAS	ZR O 2	LEFEVRE, J	63	301519
THER	ZR O 2	SCHICK, H ANTHROP	63	301580
TRT	ZR O 2	WEBER, B	62	301616
TRT	ZR O 2	BUCKLEY, J	62	301418
TRT	ZR O 2	VAHLDIEK, F ROBINS	62	301606
TRT	ZR O 2	HINZ, I DIETZEL, A	62	301473
TRT	ZR O 2	BAUN, W	63	201999
PHAS	ZR O 2	CARROLL, D	63	202014
PHAS	ZR O 2	COHEN, I SCHANER	63	202018
CRYS	ZR O 2	KOFSTAD, P RUZICKA	63	202073
MPP	ZR O 2	MCTAGGART, F	63	202101
MPP	ZR O 2	NAGARJAN, G	63	202106
VAP	ZR O 2	KIBLER, G LYON, T	63	301259
TRT	ZR O 2	MUMPTON, F ROY, R	60	301308
TRT	ZR O 2	VISHNEVSKII, I GAV	62	301373

CPL	ZR O 2	VICTOR, A DOUGLAS,	60	700949
CRYS	ZR O 2	ADAM, J ROGERS, M	59	300862
CRYS	ZR O 2	COCCO, A SCHROMEK	61	201211
CRYS	ZR O 2	VAN ARKEL, A	24	701066
CRYS	ZR O 2	KOMISSAROVA, L SIM	60	200819
CRYS	ZR O 2	STOCKER, J	61	201102
CRYS	ZR O 2	BELOV, N	60	600676
CRYS	ZR O 2	KELLER, E K ANDREE	61	300222
CTEX	ZR O 2	GRAIN, C CAMPBELL	61	601471
H	ZR O 2	VICTOR, A DOUGLAS	60	700949
MPP	ZR O 2	PIROGOV, A	62	300625
MPP	ZR O 2	YAVORSKY, P	62	201763
PHAS	ZR O 2	GRAIN, C CAMPBELL	61	601471
PHAS	ZR O 2	COLLONGUES R	61	201212
PHAS	ZR O 2	COCCO, A	59	201168
PHAS	ZR O 2	COCCO, A VIRDIS, P	61	201316
PHAS	ZR O 2	WHITNEY, E	62	301017
PHAS	ZR (2	DELIMARSKY, Y BUDE	[illegible]	300880
PHAS	ZR O 2	EVANS, P	61	201362
PHAS	ZR O 2	EVANS, P WILDSMITH	61	600768
PHAS	ZR O 2	VAHLDIEK, F LYNCH	60	600870
PHAS	ZR O 2	LYNCH, C VAHLDIEK	61	700620
PHAS	ZR O 2	SMITH, D CLEIN, C	62	201672
PHAS	ZR O 2	COHEN, I SCHANER	62	201645
REAC	ZR O 2	ARONSON, S	61	200998
REAC	ZR O 2	MCTAGGART, F	61	300338
REAC	ZR O 2	RUFF, O EBERT, F	29	900120
TCON	ZR O 2	ADAMS, M	54	600961
THER	ZR O 2	ACKERMANN, R THORN	58	601087
THER	ZR O 2	MCCLAINE, L	60	300278
TRT	ZR O 2	VAHLDIEK, F LYNCH	60	600870
TRT	ZR O 2	EVANS, P WILDSMITH	61	600768
VAP	ZR O 2	NAKATA, M MCKISSON	61	300313
ZKP	ZR O 2	ARONSON, S	61	200998
CRYS	ZR OXIDES	MAGNELI, A ANDERSO	61	201666
THER	ZR OXIDES	ORTNER, N ANDERSON	59	701066
VAP	ZR OXIDES	ORTNER, N ANDERSON	59	701066
CRYS	ZR O SYST	LICHTER, B	60	200774
THEO	ZR O SYST	FLODMARK, S ROOS	63	301219
CRYS	ZR O SYST	LICHTER, B	60	600670
ERES	ZR O SYST	WASILEWSKI, R	62	301076
ERES	ZR O SYST	GEBHART, E SAGHEZZ	61	300330
KIN	ZR O SYST	KUBASCHEWSKI, O	62	601577
PHAS	ZR O SYST	KUBASCHEWSKI, O	62	601577
MPP	ZR O SYST	DEBUIGNE, J LEHR	63	202026
PHAS	ZR O SYST	BURDESE, A BORLERA	60	200946
PHAS	ZR O SYST	HOLMBERG, B DAGERH	61	300326
THER	ZR O SYST	VEINBACHS, A KOMAR	62	601611
PHAS	ZR O CA SYST	SHKHAREVSKII, B	61	201707
THER	ZR O CL SYST	KOMISSAROVA, L PLY	60	200811
MPP	ZR O F SYST	BUSLAYEV, Y GORBUN	62	300830
PHAS	ZR PT SYST	KENDALL, E HAYS, C	61	201095
PHAS	ZR SI B SYST	PARTHE, E NORTON	60	201404
PHAS	ZR SI O SYST	KELER, E ANDREEVA	62	201888
PHAS	ZR SI O SYST	COCCO, A SCHROMEK	60	201188
PHAS	ZR TH SYST	EVANS, D	61	201254
PHAS	ZR TI NB SYST	MIKHEEV, V BELOUSO	61	300834
PHAS	ZR TI O SYST	COCCO, A SCHROMEK	60	201188
PHAS	ZR U C SYST	BENESOVSKY, F RUDY	61	301406
PHAS	ZR U O SYST	ARONSON, S CLAYTON	61	300268
CEMP	ZR U O SYST	JOHANSEN, H CLEARY	62	201882
PHAS	ZR U O SYST	VORONOV, N VOITEKH	61	201920
THER	ZR U O SYST	ARONSON,S CLAYTON	61	300258
REAC	ZR W B SYST	HELGORS Y, J	61	201887
THER	Z' X 4	NAGARAJAN, G	62	201774